NMR Methods of Quantum State Detection

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The process of amplification of a single spin state using nuclear magnetic resonance (NMR) techniques in a rotating frame is considered. Our main aim is to investigate the efficiency of various schemes for quantum detection. Results of numerical simulation of the time dependence of individual and total nuclear polarizations for 1D, 2D, and 3D configurations of the spin systems are presented.

Key words: NMR; Spin Dynamics; Nuclear Polarization; Quantum Detection.
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1. Introduction

Concerning the impellent problem in quantum state detection information processing is amplified and then the output of a protocol is measured. Recently numbers of schemes have been proposed for realizing measurements of a single quantum state [1 – 7]. These schemes will play an important role in building up a quantum device for amplification of a very low signal from a single quantum object. To estimate the efficiency of these schemes several values can be used. One of them is the contrast, C, introduced in [3, 4]:

$$C = \frac{M_z^{(0)} - M_z^{(1)}}{M_z(0)}, \tag{1}$$

where $M_z^{(0)}$ and $M_z^{(1)}$ are the nuclear magnetizations of the system obtained when the measured nuclear spin is in the state $|0\rangle$ or $|1\rangle$, respectively, and $M_z(0)$ is the initial nuclear magnetization. The quantity for contrast received within the framework of realizable model lies in a range of $1.6 \div 1.7$, while the maximum theoretical contrast is 2 [1, 3, 4].

Recently, a principle of quantum detection of the state of a single spin in a one-dimensional Ising chain was shown with nearest-neighbor interactions [1] and also in a more realistic spin system including interactions beyond the nearest neighbours and natural dipole-dipole interactions [8]. In this model, a wave of flipped spins can be triggered by a single spin flip and the polarization of the single spin is converted into a total polarization of the spin system. This process can be described by using the sequence of quantum gates [1, 5]

$$CNOT_{N,N-1} \ldots CNOT_{3,2} CNOT_{2,1}, \tag{2}$$

where $CNOT_{n,m}$ is the control-not gate, which leads to flip the state of the m-th qubit when the n-th qubit is in the state $|1\rangle$ and does not do anything when the n-th qubit is in the state $|0\rangle$. An equivalent explanation can be given by using the following physical arguments. The effective field on each spin is determined as a vector sum of the local field, ω_{d}, produced by neighbour spins and a radio-frequency (RF) field. When a spin, oriented along the Z-axis and irradiated by a weak RF field along the X-axis, $\vec{H}_1 || X$, has the two neighbours in different states, for example, one up, along an external magnetic field, $\vec{H}_0 || Z$, and another down, antiparallel to $\vec{H}_0$, the local field produced by these nearest-neighbours on the spin would have been zero. The spin starts to rotate around the direction of the weak RF field and changes its initial direction. By contrast, when a spin has two neighbours in the same state, for example along $\vec{H}_0$, the local field on this spin would have been not zero in the Z-direction. The effective field coincides with the local one so that the spin remains in the former position. Evidently, the above-mentioned explanation is correct for the simple model of a spin system with a weak dipolar coupling between nearest neighbours when a Hamiltonian includes only the Z-components of the spin operators. In real solids, the main interaction is a dipole-dipole one with coupling of all spins in a cluster, and the Hamiltonian includes all components of the spin operators.

In the present paper we consider a nuclear spin system in a rotating frame representation. The system consists of two parts. One of the parts is simply one spin (S), the state of which is detected. The second part is a system of dipolar coupling homonuclear spins, which plays the role of a measuring device. Our main goal is to convert the polarization of the target single spin into a total polarization of the spin system. First we consider one-dimensional spin systems, namely, chains and rings of spins in the limit of weak coupling [9]. For these spin systems we obtain effective Hamiltonians. Then the amplification processes are studied in two- and three-dimensional spin systems. Finally, the efficiency of this scheme is discussed.

2. Averaging of Interaction with an External Field

Let us consider the model of a system of the nuclear spin S and N spins I coupled by dipole-dipole interaction, placed in a high magnetic field, $\vec{H}_0$, directed along the Z-axis and irradiated at resonance by weak transverse RF fields, $\vec{H}_1(t) = \vec{H}_1 \cos \Omega_0 t$ and $\vec{h}_1(t) = \vec{h}_1 \cos \omega_0 t$ directed along the X-axis, where H_1 and h_1 are the amplitudes of the weak RF fields. The Hamiltonian of the spin system can be presented in the following form:

$$H_{\text{lab}} = \Omega_0 S^z + \Omega_1 S^x \cos \Omega_0 t + \omega_0 \sum_{n=1}^{N} I_n^z + \omega_1 \sum_{n=1}^{N} I_n^x \cos \omega_0 t + H_{\text{dd}} + H_{SI}, \tag{3}$$

where $\Omega_{0.1} = \gamma_S H_{0.1}$, $\omega_0 = \gamma_I H_0$ and $\omega_1 = \gamma_I h_1$, γ_S and γ_I are the gyromagnetic ratio of nuclei S and I. S^z, S^x, I_n^z and I_n^x are the angular momentum operators of S and I nuclei in the Z- and X-directions, respectively. H_{dd} is the secular part of the dipole-dipole interaction Hamiltonian with the coupling constant d_{mn} between the I nuclei:

$$H_{\text{dd}} = \sum_{m>n} d_{mn} \left[I_m^z I_n^z - \frac{1}{2} (I_m^x I_n^x + I_m^y I_n^y) \right]. \tag{4}$$

H_{SI} is the secular part of the dipole-dipole interaction Hamiltonian with the coupling constant g_m between the unlike spins I and S nuclei:

$$H_{SI} = \sum_m g_m S^z I_m^z. \tag{5}$$

In the rotating frame at $\Omega_0 \approx \omega_0 \gg d_{mn} \approx g_m \gg \omega_1 = \Omega_1$, the fast oscillating terms can be removed [10, 11]:

$$H_{\text{rot}} = \frac{\Omega_1}{2} S^x + \frac{\omega_1}{2} \sum_{n=1}^{N} I_n^x + H_{\text{dd}} + H_{SI}. \tag{6}$$

To reach our goal and convert the polarization of the spin S to the total polarization of the spin system I the Hartmann-Hahn condition [12], $\omega_1 = \Omega_1$, must be fulfilled.

Usually, at $\omega_1 = \Omega_1 \gg \omega_{\text{d}} = \sqrt{\frac{\text{Tr}(H_{\text{dd}})^2}{\text{Tr}(\sum_n I_n^z)^2}}$, the dipolar Hamiltonian, H_{dd}, can be taken into account by an averaging procedure [10, 11]. The case considered here is opposite, $\omega_1 = \Omega_1 \ll \omega_{\text{d}}$. To correctly take into account the first two terms on the right-hand side of (6) let us perform the unitary transformation of the first two terms of the Hamiltonian (4) [1]:

$$\tilde{H}(t) = \frac{\omega_1}{2} U(t) \left(S^x + \sum_{n=1}^{N} I_n^x \right) U^+(t), \tag{7}$$

where

$$U(t) = \exp[-\text{i}t(H_{\text{dd}} + H_{SI})]. \tag{8}$$

At $\omega_d \gg \omega_1$, it becomes appropriate to take into account in the lowest order the time-independent part of the Hamiltonian (7). Thus, the effective time-independent Hamiltonian can be obtained [10, 11]:

$$H_{\text{eff}}^{(0)} = H^{(0)} = \frac{1}{t_{\text{c}}} \int_0^{\text{c}} \text{d}t \tilde{H}(t). \tag{9}$$

3. Quantum State Detection

The first step of detection of a single spin state consists of in the conversion of the weak signal of the single spin to the large system, called as measuring device. It is difficult to study this process in detail because usually the devices are classical and too large and complex. To overcome these difficulties it was proposed to consider simpler and distinct models of a quantum detector with controllable spin dynamics [1 – 5]. Following these ideas and considering an ensemble of N spins with $I = 1/2$, forms a measuring device and the target single spin, $S = 1/2$ can be measured. First, the I spin system is prepared in a highly polarized state with the initial density matrix:

$$\rho(0) = \otimes_{k=1}^{N} \rho_k(0), \tag{10}$$

where $\rho_k(0) = \begin{array}{|c|c|}\hline 1 & 0 \\ \hline 0 & 0 \\ \hline \end{array}_k$ is the initial density matrix of

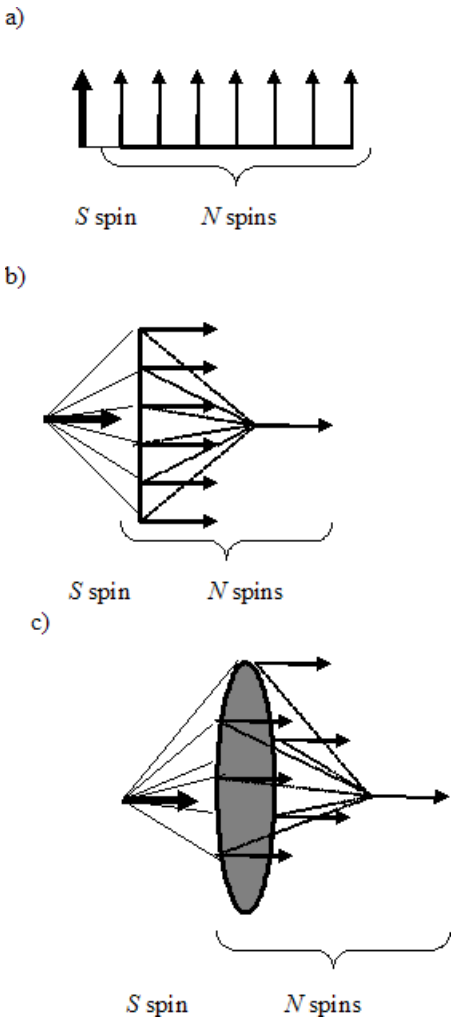

Fig. 1. Configurations of a measuring device (the ensemble of seven spins with $I = 1/2$; thin arrows) and the target spin S (thick arrow); (a) 1D system; (b) 2D system; (c) 3D system.

the k-th spin oriented *up* along the external magnetic field $\vec{H}_0$. Below we consider "measuring" spin systems design as one-, two-, and three-dimensional systems (Fig. 1).

3.1. One-Dimensional Model

Let us consider a one-dimensional (1D) linear spin chain (Fig. 1a). In the limit of weak coupling [8] the Hamiltonian describing the spin system can be presented by (3) with

$$H_{\mathrm{dd}} = \sum_{n<m}^{N} d_{mn} I_m^z I_n^z, \tag{11}$$

where $d_{mn} = d_1/(m-n)^3$ and d_1 is the coupling strength between the nearest I spins. In the rotating frame (3) becomes [10, 11]

$$H_{\mathrm{rot}} = \frac{\omega_1}{2}\left(S^x + \sum_{n=1}^{N} I_n^x\right) + \sum_{n<m}^{N} d_{mn} I_m^z I_n^z + \sum_{m}^{N} g_m S^z I_m^z, \tag{12}$$

where $g_m = g_1/m^3$ and g_1 is the coupling strength between the nearest S and I spins. The Hamiltonian (12) can be rewritten in a suitable form for further consideration [9]:

$$H = \frac{\omega_1}{2}\left(S^x + \sum_{n=1}^{N} I_n^x\right) + \sum_{q=1}^{M}\left(d_q \sum_{k=1}^{N-q} I_k^z I_{k+q}^z + g_q S^z I_q^z\right), \tag{13}$$

where $d_q = d_{k,k+q}$ are the coupling constants between the k-th and $(k+q)$-th nuclear spins, and M is a number of directed coupling spins, for example, at the nearest neighbour approximation $M = 1$ and at the next-nearest neighbour approximation $M = 2$. At $\omega_1 \ll d_q$ the first term on the right-hand side of (13) can be taken correctly into account by using the averaging procedure [1]. It is useful for this purpose to transform the first term of the Hamiltonian (13) by the unitary transformation

$$\tilde{H}(t) = \frac{\omega_1}{2} \mathrm{e}^{\left[-\mathrm{i}t\sum_{q=1}^{M}\left(d_q\sum_{k=1}^{N-q} I_k^z I_{k+q}^z + g_q S^z I_q^z\right)\right]} \cdot \left(s^x + \sum_{n=1}^{N} I_n^x\right) \mathrm{e}^{\left[\mathrm{i}t\sum_{q=1}^{M}\left(d_q\sum_{k=1}^{N-q} I_k^z I_{k+q}^z + g_q S^z I_q^z\right)\right]}. \tag{14}$$

When the modulation is very rapid compared to the magnitude, $d_q \gg \omega_1$, it becomes appropriate to take only the time-independent part of the Hamiltonian (14) into account [10, 11].

Using the transformation rules for the X-component of the spin operators,

$$\mathrm{e}^{-\mathrm{i}taAB} Q \mathrm{e}^{\mathrm{i}taAB} = Q\cos\left(\frac{at}{2}\right) + 2PB\sin\left(\frac{at}{2}\right), \tag{15}$$

and for the Y-component of the spin operators,

$$\mathrm{e}^{-\mathrm{i}taAB} P \mathrm{e}^{\mathrm{i}taAB} = P\cos\left(\frac{at}{2}\right) - 2QB\sin\left(\frac{at}{2}\right), \tag{16}$$

where $a = d_q$; $A = I_k^z$, S^z; $B = I_{k+q}^z$, I_q^z; $Q = I_k^x$, S^x; $P = I_k^y$, S^y, the effective time-independent Hamiltonian in the approximation of the nearest neighbour interacting

spins ($M = 1$) can be obtained:

$$H_{\text{eff}}^{(M=1)} = \left(\frac{g}{2}\right) S^z + \frac{\omega_1}{8} S^x (1 - 2I_1^z) - \left(\frac{d_1 + g_1}{2}\right) I_1^z + \frac{\omega_1}{8} I_1^x (1 - 2I_2^z)(1 + 2S^z) + \left(\frac{d_1}{2}\right) I_N^z + \frac{\omega_1}{8} I_N^x (1 - 2I_{N-1}^z) + \frac{\omega_1}{4} \sum_{k=2}^{N-2} I_k^x (1 - 4I_{k-1}^z I_{k+1}^z). \quad (17)$$

The effective time-independent Hamiltonian (17) has the following interpretation: the k-th spin is still at its initial state when its two neighbours are in the same state. This means that the local field produced by the $(k-1)$-th and by the $(k+1)$-th spin is doubled. When the two neighbours of the k-th spins are in different states, the local field equals zero. In this case the ensemble average $\langle 1 - 4I_{k+1}^z I_{k-1}^z \rangle = 0$. As results, the k-th spin starts to rotate around the direction of the weak RF field and changes its initial direction. The result (17) is similar to that obtained earlier [1], except for the terms with spin operators of the first and the last spins of the chain. In the case with nearest and next-nearest neighbour interactions ($M = 2$) we obtain the following expression for the effective Hamiltonian:

$$\begin{aligned} H_{\text{eff}}^{(M=2)} &= \left(\frac{g_1 - g_2}{2}\right) S^z + \left(\frac{d_2 - d_1 - g_1}{2}\right) I_1^z \\ &+ \left(\frac{d_2 - g_2}{2}\right) I_2^z - \left(\frac{d_2 t}{2}\right) i_{N-1}^z + \left(\frac{d_1 - d_2}{2}\right) I_N^z \\ &+ \frac{\omega_1}{8} S^x [(1 - 4I_2^z I_1^z) - 2(I_1^z - I_2^z)] \\ &+ \frac{\omega_1}{8} I_1^x [(1 - 4I_3^z I_1^z) - 2(I_2^z - I_3^z)](1 + 2S^z) \\ &+ \frac{1}{4} I_2^x (1 - 4I_3^z I_1^z)[(1 - 4I_4^z S^z) + 2(I_4^z S^z)] \\ &+ \frac{1}{4} I_{N-1}^x (1 + 2I_{N-3}^z)(1 - 4I_{N-2}^z I_N^z) \\ &+ \frac{\omega_1}{8} I_N^x [(1 - 4I_{N-2}^z I_{N-1}^z) - 2(I_{N-1}^z - I_{N-2}^z)] \\ &+ \frac{\omega_1}{4} \sum_{k=3}^{N-3} I_k^x (1 - 4I_{k-1}^z I_{k+1}^z)(1 - 4I_{k-2}^z - I_{k+2}^z). \end{aligned} \quad (18)$$

To estimate the efficiency of the one-dimensional scheme we calculate the time-dependences of the individual nuclear spin polarizations given by the definition

$$P_k(t) = \text{Tr}\left\{ I_k^z e^{-itH} \rho(0) e^{itH} \right\}. \quad (19)$$

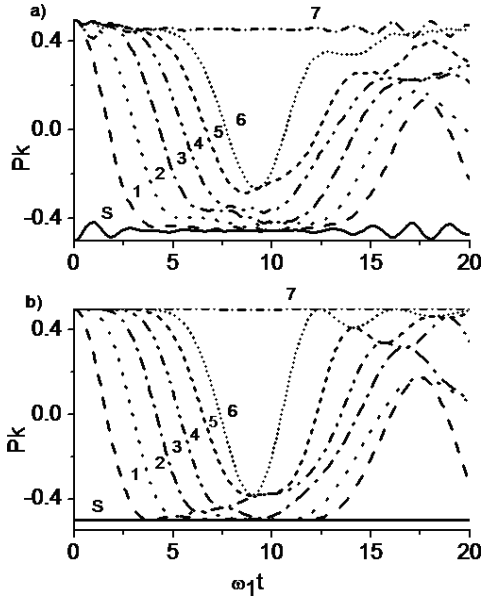

Fig. 2. Time dependences (in units of $1/\omega_1$) of the spin S state conversion to the individual polarizations of the N spin system, (a) calculated by using the Hamiltonian (13) with $M = 1$ and (b) obtained with the effective Hamiltonian (17).

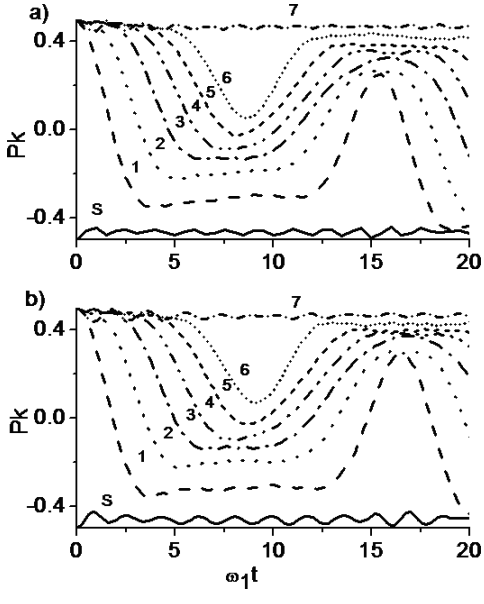

Fig. 3. (a) Time dependences of the conversion of the S spin polarization to the individual spin polarizations in a linear chain of seven dipolar-coupled spins calculated by using the Hamiltonian (13); (b) alternating chain of ^{1}H and ^{19}F nuclear spins at $\omega_1 = 0.15 D_1$.

The results of the numerical calculation for the chain with the nearest-neighbour interactions, described by

the Hamiltonian (13) with $M = 1$, are shown in Figure 2a. Spin dynamics are very close to the ones obtained with the effective Hamiltonian (17) (Fig. 2b). Including the interactions with further spins to the consideration does not cause a qualitative change in the dynamics but makes the wave somewhat less pronounced. The results for all spin couplings are shown in Figure 3a. In a chain with alternating spins of two types, irradiated by a weak RF field, the secular heteronuclear dipole-dipole Hamiltonian is changed. The interactions between equal spins are described by the Hamiltonian (4) including all components of the spin operators, while the static components remain only significant in the interaction between unequal spins; the interaction is presented by the Hamiltonian (11). As an example Fig. 3b presents the results of the calculation for a seven spin chain with alternating of hydrogen, ^{1}H, and fluorine, ^{19}F, with the gyromagnetic ratio $\gamma_{1_H} = 42.58\,\mathrm{MHz/T}$ and $\gamma_{19_F} = 40.08\,\mathrm{MHz/T}$ and $\omega_1/D_1 = 0.15$.

Note that the behaviour of the second spin is critical. Irrespective of the chain length, rotating of the second spin will lead to the propagation of a wave. Therefore, an analysis of the short spin chain with few numbers of spins gives a trustworthy information of the wave propagation in the spin chains with a large number of spins.

3.2. Two-Dimensional Model

The Hamiltonian of a two-dimensional (2D) spin system, the configuration of which is presented in Fig. 1b, has the form

$$\begin{aligned} H = {} & \frac{\omega_1}{2}\left(\sum_{m=1}^{N} I_m^x + S^x\right) \\ & + \sum_{q=1}^{M} d_q \sum_{m=1}^{N-1-q}\left[I_m^z I_{m+q}^z - \frac{1}{2}(I_m^x I_{m+q}^x + I_m^y I_{m+q}^y)\right] \\ & + \sum_{m=1}^{N-1} f_m\left[I_m^z I_N^z - \frac{1}{2}(I_m^x I_N^x + I_m^y I_N^y)\right] \\ & + \sum_{m=1}^{N-1} g_m S^z I_m^z + g_N S^z I_N^z, \end{aligned} \tag{20}$$

where f_m is the dipolar coupling constant between the N-th and m-th I nuclear spins. In the approximation of nearest neighbours the effective Hamiltonian corresponding to the two-dimensional scheme can be obtained:

$$\begin{aligned} H_{\mathrm{eff}} = \sum_{k=1}^{N-1}\Bigg\{ & \left(\frac{f_k - g_k}{2}\right) I_k^z \\ & + \frac{\omega_1}{4} I_k^x[(1 - 4I_N^z S^z) - 2(I_N^z - S^z)]\Bigg\}. \end{aligned} \tag{21}$$

The results of simulation of seven spins with $I = 1/2$ and a single spin with $S = 1/2$ in the weak coupling approximation are presented in Figure 4a. Figure 4b shows the dynamics of converting the polarization of the spin S to the polarization of the ensemble of seven spins with $I = 1/2$ described by the Hamiltonian (20) at $\omega_1 = 0.15 D_1$ with the full dipole-dipole interactions.

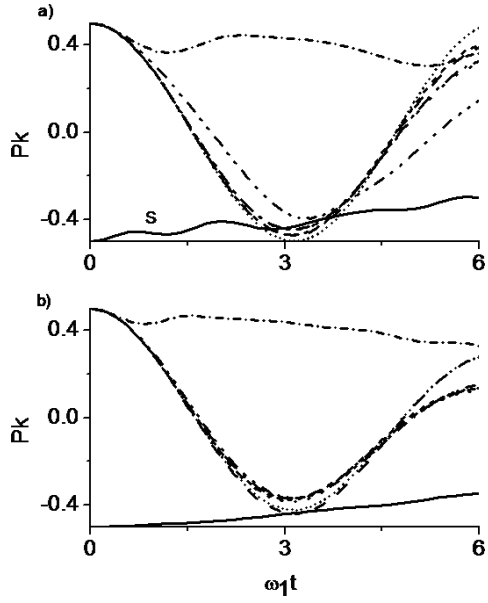

Fig. 4. Time dependences of the conversion of the S spin polarization to the individual spin polarizations in a 2D system of seven dipolar-coupled spins, (a) calculated by using the Hamiltonian (20) and (b) calculated by using the weak coupling limit.

3.3. Three-Dimensional Model

The Hamiltonian of a three-dimensional (3D) spin system, the configuration of which is presented in Fig. 1c, includes the full dipole-dipole interactions between I spins and has the form

$$H = \frac{\omega_1}{2}\left(\sum_{m=1}^{N} I_m^x + S^x\right) + D_1 \sum_{q=1}^{M}\left[\frac{\sin\left(\frac{\pi}{N}\right)}{\sin\left(\frac{\pi q}{N}\right)}\right]^3 \cdot$$

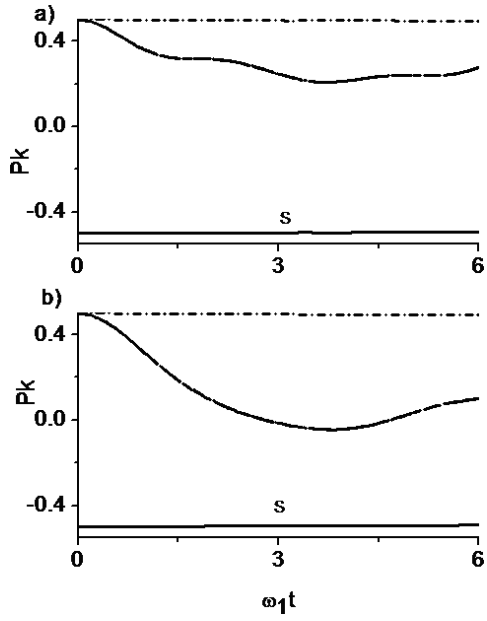

Fig. 5. Conversion of the S spin polarization to the individual spin polarizations in a 3D system of seven dipolar-coupled spins, (a) calculated by using the Hamiltonian (22) and (b) calculated by using the weak coupling limit. Six of the curves are overlapping.

$$\cdot \sum_{m=1}^{N} \left[I_m^z I_{m+q}^z - \frac{1}{2}(I_m^x I_{m+q}^x + I_m^y I_{m+q}^y) \right] + \sum_{m=1}^{N-1} R_m \left[I_m^z I_N^z - \frac{1}{2}(I_m^x I_N^x + I_m^y I_N^y) \right] + \sum_{m=1}^{N-1} Q_m S^z I_m^z + Q_N S^z I_N^z, \quad (22)$$

where R_m is the dipolar coupling constant between the N-th and m-th nuclear spin I, Q_m is the dipolar coupling constant between the spin S and the m-th nuclear spin I, and Q_n is the dipolar coupling constant between the spin S and N-th nuclear spin I. In the approximation of nearest neighbours the effective Hamiltonian corresponding to the three-dimensional scheme can be obtained:

$$H_{\text{eff}} = \frac{\omega_1}{2} \sum_{m=1}^{N-1} I_m^x \prod_{q=1}^{M} (1 - I_m^z I_{m+q}^z) + \sum_{m=1}^{N-1} R_m I_m^z I_N^z + \sum_{m=1}^{N-1} Q_m S^z I_m^z + Q_N S^z I_N^z. \quad (23)$$

Figure 5a shows the dynamics of converting the polarization of the spin S to the polarizations of the ensemble of seven spins with $I = 1/2$ in the weak coupling limit. Figure 5b presents the converting process with the full dipole-dipole interactions, described by the Hamiltonian (22) at $\omega_1 = 0.15 D_1$.

Table 1. The efficiency of amplification in one-, two-, and three-dimensional spin configurations.

		Coefficient of amplification α	Exposure T	Exposure effectiveness η	Contrast C
1D	Full d-d interaction	1.85	8.91	0.21	1.23
	Weak coupling limit	1.86	3.38	0.55	1.24
2D	Full d-d interaction	2.69	3.12	0.86	1.79
	Weak coupling limit	2.88	3.15	0.91	1.92
3D	Full d-d interaction	0.89	3.63	0.24	0.59
	Weak coupling limit	1.64	3.77	0.43	1.09

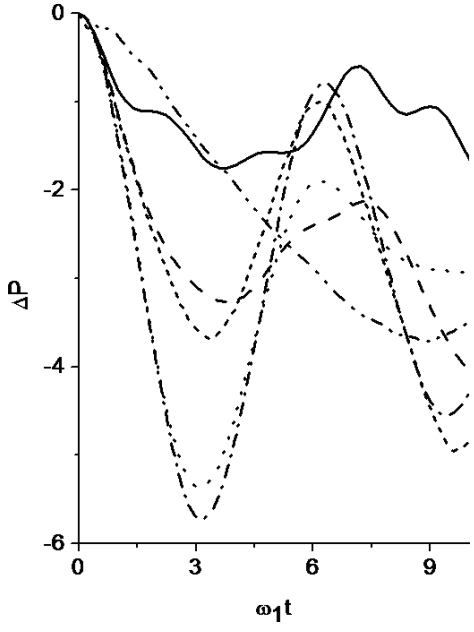

Fig. 6. Time dependences of the change in the total spin polarization, ΔP, in 3D spin system configurations with the Hamiltonian (22) (solid) and for ZZ coupling (dash); in a 2D spin system with Hamiltonian (20) (dot) and for ZZ coupling (dash-dot); and in 1D spin system configurations for the alternating spin chain with dipole-dipole couplings (dash-dot-dot) and for ZZ coupling (shot-dash).

4. Results and Discussion

The most important feature of the spin dynamics described above is signal amplification, when a state of polarization of a single spin S is converted into a total polarization of the spin system I. The change in the total polarization (magnetization) of a spin system quantifies the efficiency of this system as a quantum ampli-

fier [1 – 3]. The results for different models studied in this work are summarized in Fig. 6, which shows the time-dependences of the change in the total polarization, $\Delta P = P(t) - P(0)$, in 1D, 2D, and 3D spin system configurations. Here $P(t) = \sum_{k=1}^{N} P_k(t)$ is the total spin polarization.

The scheme will allow to estimate the efficiency of the measurement of very weak signals according to the number of parameters which characterize: 1) the coefficient of amplification, $\alpha = \frac{|\Delta P|}{2}$ [1]; 2) the time of exposure, T (in units of $1/\omega_{\rm l}$); and 3) the exposure effectiveness, $\eta = \frac{C}{T}$. The time of exposure can be defined as the time required for the achievement of the maximum contrast, but under the condition that $\omega_{\rm l} \ll \omega_{\rm d}$. Taking the influence of the relaxation and the decoherence processes into account it is useful in a real spin system to estimate the effectiveness of various quantum amplifiers using the rate of achievement of the maximal contrast, the exposure effectiveness η.

The coefficient of amplification α and the exposure time T have been extracted from Figure 6. Results are presented in Table 1.

From the table we can see that the 2D configuration of the spin system gives the largest coefficients of amplification and the smallest exposure times. Another related characteristic is the contrast C [2, 3], which is a relative change of polarization of the spin system. Its maximum possible value is $C = 2$ [1 – 3]. In models considered here the largest value of the contrast is reached in the 2D configuration of the spin system.

5. Conclusions

We have studied the process of conversion of the polarization of the nuclear single spin to the total polarization of an ensemble of nuclear spins in 1D, 2D, and 3D nuclear spin systems. It has been demonstrated that efficient amplification dynamics can be organized for natural dipole-dipole couplings, both in the weak coupling limit and full dipole-dipole interactions. Numerical calculations are used to compare the contributions of nearest and remote spins to the conversion processes in the 1D, 2D, and 3D configuration of the spin systems.

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