Available online at www.sciencedirect.com
ScienceDirect
Solid State Nuclear Magnetic Resonance 32 (2007) 71–77
Solid State Nuclear Magnetic Resonance
www.elsevier.com/locate/ssnmr

NMR method for amplification of single-spin state

Gregory B. Furman[a,b,*], Victor M. Meerovich[a], Vladimir L. Sokolovsky[a]

[a]Physics Department, Ben-Gurion University, P.O.B. 653, Building 62, Room 104, Beer Sheva 84105, Israel
[b]Ohalo College, P.O.B. 222, Qazrin 12900, Israel

Received 7 April 2007; received in revised form 28 August 2007
Available online 14 September 2007

Abstract

Amplification of a single-spin state using nuclear magnetic resonance (NMR) techniques in a rotating frame is considered. The 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.

PACS: 76.60.−k

Keywords: NMR; Spin dynamics; Nuclear polarization; Quantum detection

1. Introduction

The impellent problem in quantum information processing concerns amplifying and then measuring the output of a protocol. Recently, many schemes have been proposed for realizing of 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 magnetization of the system obtained when the measured nuclear spin is in the state $|0\rangle$ or $|1\rangle$, respectively, $M_z(0)$ is the initial nuclear magnetization. Quantity for contrast received within the framework of the realizable models lies in a range 1.6–1.7, while the maximum theoretical contrast is 2 [1,3,4].

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

$$\mathrm{CNOT}_{N,N-1} \ldots \mathrm{CNOT}_{3,2}\mathrm{CNOT}_{2,1}, \tag{2}$$

where $\mathrm{CNOT}_{n,m}$ is the control-not gate, which leads to flip the state of the mth qubit when the nth qubit is in the state $|1\rangle$ and does not do anything when the nth qubit is in the state $|0\rangle$. The equivalent explanation can be defined 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 neighbor spins, and radio-frequency field (RF). When a spin, oriented along Z-axis and irradiated by a weak RF field along X-axis, $\vec{H}_1 || X$, has the two neighbors in different states, for example, one up, along an external magnetic field, $\vec{H}_0 || Z$, and another down, anti-parallel to $\vec{H}_0$, the local field produced by these nearest neighbors on the spin equals to zero. The spin starts to rotate around the direction of the weak RF field and changes its initial direction. In contrast, when a spin has two neighbors in the same state, for example along $\vec{H}_0$, the

*Corresponding author. Physics Department, Ben-Gurion University, P.O.B. 653, Building 62, Room 104, Beer Sheva 84105, Israel. Fax: +972 8 6472 903.
E-mail address: gregoryf@bgu.ac.il (G.B. Furman).

0926-2040/$ - see front matter © 2007 Published by Elsevier Inc.
doi:10.1016/j.ssnmr.2007.08.003

local field on this spin is not zero in the Z direction. The effective field coincides with the local one with the result that the spin remains in the former position. Evidently, the above-mentioned explanation is correct for the simple model of spin system with a weak dipolar coupling between nearest neighbors 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 all spins in a cluster, and the Hamiltonian includes all components of spin operators. The previous proposed methods for single-spin measurements concentrate on the linear chain (1D) [1,8] and cubic (3D) [6] spin systems.

In the present paper we compare the efficiency of the 1D, 2D, and 3D configuration of the spin systems to realize a single-spin measurement scheme. The advantage of 2D and 3D configurations over the previous schemes [1,6,8] is that all spins have the same possibility to be flipped simultaneously. We consider a nuclear spin system in a rotating frame representation. The system consists of two parts. One of the parts is simple one spin (S), state of which is detected. The second part is a system of dipolar coupling homonuclear spins, which plays a role in the measuring device. Our main goal is to convert the polarization of the target single-spin (S) 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]. Then the amplification processes are studied in two- and three- dimensional spin systems. Finally, we discuss the efficiency of these schemes. We suggest that internal spin dynamics, with natural dipole–dipole interaction, can serve as a "pre-detector" for producing stronger signals, and may even help in reaching the ultimate limit of a single-spin detection by using clusters of coupled nuclear spins and conventional NMR techniques and spectrometers.

2. Average Hamiltonian

Let us consider the model of a system of 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 on resonance by weak transverse RF fields, $\vec{H}_1(t) = \vec{H}_1 \cos \Omega_0 t$ and $\vec{h}_1(t) = \vec{h}_1 \cos \omega_0 t$, 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:

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

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 I nuclei

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

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

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

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

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

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 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 in the right-hand side of Eq. (6) let us perform the unitary transformation of the first two terms of 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

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

At $\omega_{\text{d}} \gg \omega_1$ in the lowest order the time-independent part of Hamiltonian (7), the effective time-independent Hamiltonian can be obtained [10,11]

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

3. Quantum-state detection

Let us consider the ensemble of $N+1$ spins consists of N spins $I = \frac{1}{2}$ and a single-spin, $S = \frac{1}{2}$. The I-spin system will be considered as a measuring device while the S spin will be regard as a target single-spin. 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 $\rho_k(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_k$ is the initial density matrix of the kth spin oriented up, along the external magnetic field $\vec{H}_0$. The