

# The qubit states decoherence in antiferromagnet-based nuclear spin model of quantum register

Alexander A.Kokin<sup>1\*</sup> and Vladimir A.Kokin<sup>2</sup>

<sup>1</sup>Institute of Physics and Technology of RAS, 34, Nakhimovskii pr., 117218 Moscow, Russia;

<sup>2</sup>Institute of Radioengineering and Electronics of RAS, 11, Mokhovaya str., 103907, Moscow, Russia

## Abstract

This study deals with the further development of nuclear spin model of scalable quantum register, which presents the one-dimensional chain of the magnetic atoms with nuclear spins 1/2, substituting the basic atoms in the plate of nuclear spin-free easy-axis 3D antiferromagnet. The decoherence rates of one qubit state and entanglement state of two removed qubits and longitudinal relaxation rates are caused by the interaction of nuclear spins-qubits with virtual spin waves in antiferromagnet ground state were calculated. It was considered also one qubit adiabatic decoherence, is caused by the interaction of nuclear spin of quantum register with nuclear spins of randomly distributed isotopes, substituting the basic nuclear spin-free isotopes of antiferromagnet. We have considered finally encoded DFS (Decoherence-Free Subspaces) logical qubits are constructed on clusters of the four-physical qubits, given by the two states with zero total angular momentum.

**Keywords:** Easy-axis antiferromagnet, decoherence, indirect coupling, inhomogeneous magnetic field, nuclear spin, quantum register and qubit.

PACs: 75.10.Pq, 75.50.Ee, 76.60.-k, 82.56.-b.

## 1 Introduction

In early papers [1-4], we have considered a model of NMR quantum register, which is based on the nuclear spin-free easy-axis 3D antiferromagnet at low temperature in homogeneous field. It was shown that the range of indirect coupling can ran up to a great value close to critical point of spin-flop quantum phase transition in antiferromagnet. We have extended the previous model into the case of inhomogeneous external magnetic field.

It was proposed to use the natural antiferromagnetic crystals with easy-axis anisotropy as an antiferromagnet thin plate (or film). As examples, they may be crystals  $\text{CeC}_2$  with tetragonal and  $\text{FeCO}_3$  (siderite) with trigonal symmetry. The basic isotopes of these crystals  $^{12}\text{C}$ ,  $^{56}\text{Fe}$  (91.7%),  $^{16}\text{O}$ ,  $^{140,142}\text{Ce}$  (99.6%) have no nuclear spins (in brackets percent isotopic abundance is given). To form the one-dimension nuclear spin chains the isotopic substitution atoms, such as  $^{12}\text{C}$  in corresponding crystal lattice sites, for isotopes  $^{13}\text{C}$  with nuclear spins 1/2, are proposed. One would expect that period of such solid state NMR quantum registers may be much more than periods of crystal lattice.

The simple antiferromagnet model to be studied here consists of two incorporated to each other tetragonal magnetic sublattices **A** and **B** with  $N = N_{\perp}N_z$  sites in each sublattice, where  $N_{\perp} = N_xN_y \gg 1$  are the sites numbers in plane of plate ( $x,y$ -axes) and  $N_z > 1$  is the sites numbers in  $z$  direction. The atom sites of sublattices are numbered respectively by numbers  $j$  and  $i$ . Each sublattice constant in the plane of the plate is  $a_{\perp}$  and along symmetry axis is  $a_z$ .

The external magnetic field  $B(x)$  in considered model (Fig. 1) is directed parallel to  $z$ -axis and to the antiferromagnet easy axis. It is assumed here, that the field gradient is of the order  $dB_z(x)/dx = G \sim 0.1 \text{ T}/\mu\text{m}$  ( $x$ -axis in plane of the plate along nuclear spin chain). This value of the gradient corresponds to the difference of resonance frequencies of the order of 100 kHz for two nuclear spins, being separated by  $100 a_{\perp}$  ( $a_{\perp} \sim 1 \text{ nm}$ ).

The qubits number in quantum register will be limited by planar structure dimensions. For example, the structure with linear dimension of the order of  $10 \mu\text{m}$  will have 100 qubit register with period  $L = 100 a_{\perp}$ .

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\*E-mail: aakokin@mail.ru

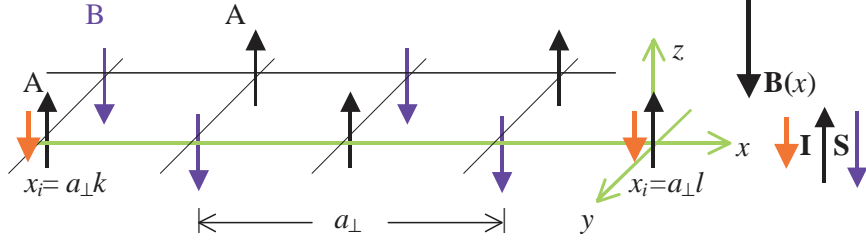


Figure 1: The scheme of antiferromagnet based nuclear spin quantum register in external field lower than critical field for spin-flop phase transition  $B(x) \ll B_C$ . The oriented (that is nonprecessing) arrows represent here the ground states of corresponding individual Bloch vectors. The nuclear spins  $\mathbf{I}_A$  (shot red arrows) are contained here only in atoms of sublattice **A**.

The starting spin Hamiltonian of 3D easy-axis antiferromagnet with interaction only between neighbouring atoms, which belong to the distinct sublattice, is represented for our model as

$$H_S = \gamma_S \hbar \left( \sum_i^N B(x_i) S_{Az}(r_i) + \sum_j^N B(x_j) S_{Bz}(r_j) \right) + \quad (1)$$

$$+ 2\gamma_S \hbar / Z \sum_i^N \sum_\delta^Z \{ B_E S_A(r_i) S_B(r_i + r_\delta) + B_A S_{Az}(r_i) S_{Bz}(r_i + r_\delta) \},$$

where  $S_A(r_i)$  and  $S_B(r_i + r_\delta)$  are electron spin operators ( $S = 1/2$ ) for neighbouring sites of sublattices **A** and **B**,  $B(x_i) = B + Gx_i$ ,  $B$  is the field value at the origin of the coordinates  $x_i$ ,  $Z = 6$  is the number of neighbouring atoms for tetragonal sublattice,  $\gamma_S = 175.88 \text{ rad GHz/T}$  ( $\gamma_S/2\pi = 28 \text{ GHz/T}$ ) is electron spin gyromagnetic ratio,  $\hbar = 1.054 \cdot 10^{-34} \text{ Js/rad}$ .

The direct product of spin operators in Eq.(1) written in matrix representation is common designated by symbol  $\otimes$ . In the following this symbol will be for brevity omitted.

In Eq.(1) the parameters  $B_E \sim (10 - 100) \text{ T}$ ,  $B_A \sim (10^{-2} - 1) \text{ T} > 0$ ,  $B_C = \sqrt{2B_E B_A + B_A^2}$  are exchange field, anisotropy and critical spin-flop field for easy-axis antiferromagnet (particularly, for  $\text{FeCO}_3$ :  $B_E = 35 \text{ T}$ ,  $B_A = 3.3 \text{ T}$   $B_C \approx 15.5 \text{ T}$ ).

It was shown in Ref.[1-4], that indirect interaction of two nuclear spins in the model of antiferromagnet-based nuclear spin quantum register with inhomogeneous magnetic field essentially grows and qualitatively changes its character, if the value of local field in the mid point of two considered nuclear spin is close to the critical field for quantum phase transition of spin-flop type in bulk easy-axis antiferromagnet. The corresponding coordinates of nuclear spins were named by us as turning points.

In present paper, we have presented the further investigations and development of this model. With the more refined results of the model analysis it was investigated here in details the one-qubit and two-qubit nonadiabatic decoherence and longitudinal relaxation rates are caused by the interaction of nuclear spins with virtual spin waves in antiferromagnet ground state. It was considered also one qubit adiabatic decoherence, is caused by the interaction with nuclear spins of randomly distributed isotopes, substituting the nuclear spin-free isotopes of basic antiferromagnet. We have considered finally, as an example, encoded DFS (Decoherence-Free Subspaces)-states of logical qubits are constructed on clusters of the four-physical qubits, given by the two states with zero total angular momentum.

The paper is organized as follows. In Section 2 we have considered some general expressions of one qubit decoherence and relaxation processes are caused by interaction of nuclear spin with spin waves in easy axis antiferromagnet plate with inhomogeneous magnetic field. In Section 3 it was considered the nonadiabatic one qubit decoherence and longitudinal relaxation. In Section 4 it was considered the decoherence of two qubit entangled quantum states. In Section 5 we have considered the adiabatic decoherence is caused by interaction with nuclear spins of random distributed isotopes, substituting the spin-free atoms of basic antiferromagnet. In Section 6 we have discussed an encoded DFS (Decoherence-Free Subspaces)-states of logical qubits on clusters of the four-physical qubits. In Conclusion we discuss the some prospects of considered quantum register model.

## 2 Some general expressions for one qubit decoherence and longitudinal relaxation in antiferromagnet-based quantum register

The antiferromagnet electron spin system of considered model plays the role of an environment for nuclear spin quantum register, whose interaction with spin wave leads on the one hand, to indirect coupling between nuclear spins and on the other hand to decoherence and relaxation processes of their states.

Let us consider the decoherence and relaxation processes of quantum state for single nuclear spin placed at position  $k$  on axes  $x$  of sublattice  $\mathbf{A}$  which is caused by its interaction with virtual magnon excitation in antiferromagnet. Such processes are described by transverse and longitudinal relative to external field components of Bloch vector (Ref.[5])

$$P^-(k, \tau) = (P^+(k, \tau))^* = P_x(k, \tau) - iP_y(k, \tau) = 2 \text{Tr} (I^-(k) \rho(k, \tau)) = 2 \text{Tr}_I (I^-(k) \rho_I(k, \tau))$$

$$P_z(k, \tau) = 2 \text{Tr}_I (I_z(k) \rho_I(k, \tau)), \text{Tr}_I I_z^2 = 1/2, \text{Tr}_I I^+ I^- = 1, \quad (2)$$

where non-steady reduced to one nuclear spin density matrix in antiferromagnet is represented by

$$\rho_I(k, \tau) = 1/2 [1 + P_z(k, \tau) I_z(k, \tau) + P^-(k, \tau) I^+(k, \tau) + P^+(k, \tau) I^-(k, \tau)] \quad (3)$$

Let us pass next in Eq. (1) to dimensionless designations:

$$h_S = H_S/\hbar\omega_E, \gamma_S B_E = \omega_E, 0 < B_A/B_E = b_A < 1, 0 < B/B_E = b, G a_{\perp}/B_E = g \sim 10^{-5}. \quad (4)$$

The interaction of  $k$ -th nuclear spin with external magnetic field and magnon excitations will be described here by dimensionless Hamiltonian with hyperfine interaction of the form (Ref.[4])

$$\begin{aligned} h &= H/\hbar\omega_E = h_S - (\omega_I(k) - a S_z(k)) I_z(k) + a/2 (I^+(k) S^-(k) + I^-(k) S^+(k)) = \\ &= h_S - (\omega_I(k) - a(1/2 - \psi) I_z(k) + \Delta h_{IS}(k)), \end{aligned} \quad (5)$$

where  $I_z, I^{\pm} = I_x \pm iI_y, S_z, S^{\pm} = S_x \pm iS_y$  are nuclear and electron spin operators,  $\omega_I(k) = (\gamma_I/\gamma_S) b_k$  is resonance nuclear frequency in local field  $b_k \equiv b + gk, \gamma_I/\gamma_S \sim 10^{-3}, a = A/\omega_E \sim 10^{-3} - 10^{-4}$  is isotropic dimensionless constant of hyperfine interaction and

$$\langle 0|1/2 - S_z(k)|0\rangle \approx \langle 0|S^+(k) S^-(k)|0\rangle = \psi(k) \ll 1. \quad (6)$$

is known as ‘‘spin contraction’’.

The perturbation Hamiltonian, corresponding to the relaxation and decoherence processes in isotopic pure antiferromagnet, has the form

$$\Delta h_{IS}(k) = \Delta h_{IS}^{(1)}(k) + \Delta h_{IS}^{(2)}(k), \quad (7)$$

where

$$\Delta h_{IS}^{(1)}(k) = a/2 (I^+(k) S^-(k) + I^-(k) S^+(k)) \quad (8)$$

The second term in Eq.(7)

$$\Delta h_{IS}^{(2)}(k) = a I_z(k) (S_z(k) - \langle 0|S_z(k)|0\rangle) \approx -a I_z(k) (S^-(k) S^+(k) - \psi) \quad (9)$$

describes two-magnon interaction, which is similar to two-phonon interaction (Ref.[5],§3.4). This mechanism causes in particular the modulation of nuclear spin resonance frequency without changing its state (adiabatic decoherence). It leads to the temperature depending decoherence rate, which is negligible small at  $(b_C - b \gg \frac{k_B T}{\hbar\gamma_S B_C})$ , when the system is close to ground state. Therefore, we will neglect next the contribution of terms  $\Delta h_{IS}^{(2)}(k)$  and will use as the perturbation Hamiltonian only the expression  $\Delta h_{IS}(k) = \Delta h_{IS}^{(1)}(k)$ . In this case, relaxation of transverse component of Bloch vector is accompanied by nuclear spin flopping (nonadiabatic decoherence). At the same time, the relaxation of longitudinal component of Bloch vector also occurs. Thus, these two processes may be considered here as one unified process of nuclear quantum state damping.

We assume now that interaction of nuclear spin, which is initially at coherent state (with nonzero nondiagonal elements of density matrix  $\rho_I(k, 0)$ ), and antiferromagnet in ground state, is turning on at the initial moment  $\tau = 0$ , when nonperturbed density matrix is represented as direct product  $\rho(k, 0) = \rho_I(k, 0) \rho_S(0) = \rho_I(k, 0) |0\rangle\langle 0|$ .

Let us go next to interaction representation for density matrix relatively to Hamiltonian  $h_0(k) = h_S - (\omega_I(k) - a/2) I_z(k)$ :

$$\rho_{in}(k, \tau) = \exp(ih_0(k)\tau) \rho(k, \tau) \exp(-ih_0(k)\tau) \quad (10)$$

and to the equation for density matrix of nucleus-electron system

$$i\partial\rho_{in}(k, \tau) / \partial\tau = [\Delta h_{IS}(k, \tau), \rho_{in}(k, \tau)], \quad (11)$$

where

$$\Delta h_{IS}(k, \tau) = \exp[ih_0(k)\tau] \Delta h_{IS}(k) \exp[-ih_0(k)\tau] = \quad (12)$$

$$= a/2 \exp(-i(\omega_I(k) - a/2)\tau) I^+(k) S^-(k, \tau) + H.c.$$

It is follows from Eq.(11) in the second order of perturbation theory

$$i\partial\rho_{in}(k, \tau) / \partial\tau \approx [\Delta h_{IS}(k, \tau), \rho(k, 0)] - i \int_0^\tau [\Delta h_{IS}(\tau, k), [\Delta h_{IS}(k, \tau'), \rho(k, 0)]] d\tau'. \quad (13)$$

Let us write the derivative of expression (2) with respect to time, by using Eq.(13) and perform then the cyclic permutation under tracing. Finally, accounting the relation  $\text{Tr}([I^-(k), \Delta h_{IS}(k, \tau)] \rho_S(0)) = 0$ , we will find

$$\partial [P^-(k, \tau) \exp(i(\omega_I(k) - a(1/2))\tau)] / \partial\tau = 2 \text{Tr}\{I^-(k) \partial\rho_{in}(k, \tau) / \partial\tau\} \approx \quad (14)$$

$$\approx -2 \text{Tr}\left\{ \int_0^\tau [[I^-(k), \Delta h_{IS}(k, \tau)], \Delta h_{IS}(k, \tau')] \rho(k, 0) \right\} d\tau'.$$

By defining the transverse Bloch vector component in the form

$$P^-(k, \tau) = P^-(k, 0) \exp[-i(\omega_I(k) - a/2)\tau - \gamma_\perp(k, \tau)], \quad (15)$$

we will have:

$$d [P^-(k, \tau) \exp(i(\omega_I(k) - a/2)\tau)] / d\tau = \quad (16)$$

$$= -d\gamma_\perp(k, \tau) / d\tau \cdot P^-(k, \tau) \exp(i(\omega_I(k) - a/2)\tau),$$

where  $\text{Re} \gamma_\perp(\tau)$  is decoherence decrement and  $\text{Im} \gamma_\perp(\tau)$  is phase shift.

We will represent the nuclear density matrix in the right part of Eq.(14) by expression

$$\rho_I(k, 0) \approx 1/2\{1 + 2P_z(k, 0) I_z(k) + P^-(k, 0) I^+(k) + P^+(k, 0) I^-(k)\} |0\rangle\langle 0|. \quad (17)$$

Using in Eq.(14) the perturbation Hamiltonian (8), ignoring the factors  $\exp(\pm i(\omega_I(k) - a/2)\tau)$  and taking in the context of second order of perturbation theory in the left-hand side of Eq.(16)  $P^-(k, \tau) \approx P^-(k, 0)$ , for the decoherence rate we will obtain

$$d \text{Re} \gamma_\perp(k, \tau) / d\tau = \text{Re} \text{Tr}_I \int_0^\tau \langle 0 | [[I^-(k), \Delta h_{IS}(k, \tau)], \Delta h_{IS}(k, \tau')] I^+(k) | 0 \rangle d\tau' = \quad (18)$$

$$= \frac{a^2}{4} 2 \text{Re} \int_0^\tau \langle 0 | S^-(k, \tau) S^-(k, \tau') + S^+(k, \tau') S^-(k, \tau) | 0 \rangle d\tau'.$$

Let us consider next the relaxation longitudinal component of Bloch vector. We will write:

$$\partial P_z(k, \tau) / \partial \tau = 2 \text{Tr} I_{kz} \partial \rho_{in}(k, \tau) / \partial \tau \approx \quad (19)$$

$$\approx -\text{Re} 2 \text{Tr} \int_0^\tau [[I_{kz}, \Delta h_{IS}(k, \tau)], \Delta h_{IS}(k, \tau')] \rho_I(k, 0) |0\rangle \langle 0| d\tau'.$$

Taking  $P_z(k, \tau) = P_z(k, 0) \exp(-\gamma_{\parallel}(k, \tau))$ , in the second order of the perturbation theory we will obtain:

$$dP_z(k, \tau) / d\tau \approx -d\gamma_{\parallel}(k, \tau) / d\tau \cdot P_z(k, 0), \quad (20)$$

where the longitudinal relaxation rate is

$$d\gamma_{\parallel}(k, \tau) / d\tau = (d\gamma_{\parallel}(k, \tau) / d\tau)^* = \quad (21)$$

$$= 2 \text{Re} \text{Tr}_I \int_0^\tau \langle 0 | [[I_z(k), \Delta h_{IS}(k, \tau)], \Delta h_{IS}(k, \tau')] I_z(k) |0\rangle d\tau'.$$

As a result of Eq.(21) we will have

$$d\gamma_{\parallel}(k, \tau) / d\tau \approx \quad (22)$$

$$\approx \frac{a^2}{4} 2 \text{Re} \int_0^\tau \langle 0 | S^-(k, \tau) S^+(k, \tau') + S^+(k, \tau') S^-(k, \tau) |0\rangle d\tau' = \text{Re} d\gamma_{\perp}(k, \tau) / d\tau,$$

whence it follows that for the considered mechanisms the rate of relaxation of longitudinal component is equal to the rate of relaxation of transverse component (decoherence rate).

### 3 Nonadiabatic decoherence and longitudinal relaxation rates of one qubit quantum states

For the calculation of nonadiabatic one qubit decoherence and longitudinal relaxation rates we used next the results of antiferromagnet Hamiltonian diagonalization, obtained in Ref.[4]. The transverse components of electron spin operators will take the form

$$S^-(k, \tau) = (S^+(k, \tau))^{\dagger} = \quad (23)$$

$$= \frac{1}{(2\pi)} \int [u^*(q_{\perp}, E) \exp(iE_{-}\tau) \xi^{+}(q_y, E_{-}) + v(q_{\perp}, E) \exp(-iE_{+}\tau) \xi(q_y, E_{+})] \exp(iq_x k) dE dq_{\perp},$$

where  $\xi^{+}(q_y, E_{-})$ ,  $\xi(q_y, E_{+})$  are operators of creation and annihilation of spin magnons for two branches of magnon states, which propagate along direction  $x$ -axis with dimensionless energies  $E_{\pm} = E \pm b$ ,  $E$  is a continuous energy parameter, and wave vector component  $q_y$  in the range of  $q_y$  to  $q_y + dq_y$ . The transformation coefficients have here the following asymptotic form (Ref.[4])

$$u^*(q_{\perp}, E) = \frac{1}{\sqrt{4\pi g}} \sqrt{\frac{\sqrt{1+b_C^2}}{E} + 1} \cdot \exp \left[ \frac{i}{g} \left( E q_x - \int_0^{q_x} E(q_{\perp}) dq_x \right) \right] + O(g), \quad (24)$$

$$v^*(q_{\perp}, E) = \frac{1}{\sqrt{4\pi g}} \sqrt{\frac{\sqrt{1+b_C^2}}{E} - 1} \cdot \exp \left[ \frac{i}{g} \left( E q_x - \int_0^{q_x} E(q_{\perp}) dq_x \right) \right] + O(g),$$

where  $b_C = B_C/B_A$  is dimensionless critical field of phase transition and  $E(q_\perp) \approx \sqrt{b_C^2 + \frac{q_\perp^2}{12}}$ .

Let us restrict next to low magnon excitation mode with energy  $E_-$ . Further, let us insert weak magnon damping  $s$  ( $E_- \rightarrow E_- + is$ ,  $E_- \gg s > 0$ ) and make a set of rearrangements, after which we will obtain

$$\text{Re } d\gamma_\perp(k, \tau) / d\tau \approx \quad (25)$$

$$\approx \frac{a^2}{(4\pi)^2} \text{Re } 2 \int_0^\tau \int u^*(q_\perp, E) u(q'_x, q_y, E) \exp(-(iE_- - s)(\tau' - \tau)) \exp(i(q_x - q'_x)k) dq'_x dq_\perp dE d\tau'.$$

For the estimation of magnon damping it may be used the line width of antiferromagnetic resonance  $s \sim \gamma_S \Delta B / \omega_E$ . The typical value of AFR line width is  $\Delta B \sim 10^{-4}$  T and  $s \sim \Delta B / B \sim 10^{-5}$ .

Upon integrating over  $\tau'$ , we have

$$\text{Re } d\gamma_\perp(k, \tau) / d\tau \approx \quad (26)$$

$$\approx \frac{a^2}{(4\pi)^2} \text{Re } 2 \int u^*(q_\perp, E) u(q'_x, q_y, E) \exp(i(q_x - q'_x)k) \frac{1 - \exp((iE_- - s)\tau)}{-iE_- + s} dE dq_\perp dq'_x.$$

By using the expression  $E(q_\perp) \approx \sqrt{b_C^2 + \frac{q_\perp^2}{12}}$ , we write

$$dq_\perp = 2\pi q_\perp dq_\perp = 24\pi E(q_\perp) dE(q_\perp), \quad 0 < q_\perp \leq \pi \quad (27)$$

and take notations  $\Delta b_k = b_C - b - gk$ ,  $\xi = E(q_\perp) - b_C$ . Upon integrating over  $E$  and  $q'_x$  (Ref.[4]), we will transform Eq.(26) for decoherence rate to the form

$$\text{Re } d\gamma_\perp(k, \tau) / d\tau = \frac{3a^2}{2\pi} R_\perp(\Delta b_k, \tau) = \quad (28)$$

$$= \frac{3a^2}{2\pi} \int_0^{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C} \left( \sqrt{1 + b_C^2} + b_C + \xi \right) Y(\xi, +\Delta b_k, \tau) d\xi,$$

where

$$Y(\xi + \Delta b_k, \tau) = \text{Re} \frac{1 - \exp[(i(\xi + \Delta b_k) - s)\tau]}{-(i(\xi + \Delta b_k) - s)} = \quad (29)$$

$$= \frac{(\xi + \Delta b_k) \sin((\xi + \Delta b_k)\tau) \exp(-s\tau)}{(\xi + \Delta b_k)^2 + s^2} + s \frac{1 - \cos((\xi + \Delta b_k)\tau) \exp(-s\tau)}{(\xi + \Delta b_k)^2 + s^2}$$

For the case of  $\Delta b_k \gg s > 0$ , after omitting  $s^2$  in dominator the Eq.(28) take the following explicit form.

$$R_\perp(\Delta b_k, \tau) \approx \left\{ \left( \sqrt{1 + b_C^2} + b_C - \Delta b_k \right) \left[ \text{si}(\Delta b_k \tau) - \text{si} \left( \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right) \tau \right) \right] + \right.$$

$$\left. + 1/\tau \left[ \cos(\Delta b_k \tau) - \cos \left( \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right) \tau \right) \right] \right\} \exp(-s\tau) +$$

$$+ s \left( \sqrt{1 + b_C^2} + b_C - \Delta b_k \right) \left\{ \frac{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C}{\Delta b_k \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right)} \left[ \frac{\cos(\Delta b_k \tau)}{\Delta b_k} - \frac{\cos \left( \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right) \tau \right)}{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k} \right] + \right.$$

$$\left. + \tau \left( \text{si}(\Delta b_k \tau) - \text{si} \left( \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right) \tau \right) \right) \right\} \exp(-s\tau) \quad (30)$$

$$+s \left\{ \log \frac{\left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right)}{\Delta b_k} + \left[ \text{ci}(\Delta b_k \tau) - \text{ci} \left( \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k \right) \tau \right) \right] \exp(-s\tau) \right\} > 0,$$

where  $\text{si}(x) = -\int_x^\infty \frac{\sin t}{t} dt$ ,  $\text{ci}(x) = -\int_x^\infty \frac{\cos t}{t} dt$  are sine-integral, and cosine-integral, and  $\lim_{\tau \rightarrow 0} [\text{ci}(a\tau) - \text{ci}(b\tau)] = \log \frac{a}{b}$ .

Fig. 2 gives the  $\tau$ -dependence of  $R_\perp(\Delta b_k, \tau)$  for distinct values of parameter  $\Delta b_k$ .

We notice, that oscillating part of the rate of decoherence tends fast (microseconds) to constant.

Taking then  $\tau \rightarrow \infty$  ( $\tau \gg 1/s \sim 10^5$ ), we will obtain for inverse time of decoherence

$$\begin{aligned} 1/T_D &= \omega_E \text{Re } d\gamma_\perp(k, \infty) / d\tau = \omega_E \frac{3a^2}{2\pi} R_\perp(b_k, \infty) = \\ &= \omega_E s \frac{3a^2}{2\pi} \left\{ \frac{\left( \sqrt{1+b_C^2} + b_C - \Delta b_k \right) \left( \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C \right)}{\Delta b_k \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k} + \log \frac{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k}{\Delta b_k} \right\}. \end{aligned} \quad (31)$$

For values  $a^2 \sim 10^{-6} - 10^{-8}$ ,  $s \sim 10^{-5} \ll \Delta b_k \ll 1_k$ ,  $\omega_E/2\pi \sim 10^{11}$  Hz decoherence time is  $T_D \sim \Delta b_k / \omega_E s a^2$  sec.

It follows that decoherence time, caused by one-magnon processes near turning points tends fast to the low value (for  $\Delta b_k \geq 10^{-3}$  decoherence time may be from milliseconds to seconds). Note that character of nonadiabatic decoherence rate depends on the anisotropy of antiferromagnet (through parameter  $b_C$ ) and from inhomogeneity of external field (through parameter  $\Delta b_k$ ).

The expression for frequency shift is

$$\begin{aligned} \text{Im } d\gamma_\perp(k, \infty) / d\tau &= \\ &= -\frac{3a^2}{2\pi} \left\{ \left( \sqrt{1+b_C^2} + b_C - \Delta b_k \right) \log \frac{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C + \Delta b_k}{\Delta b_k} + \sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C \right\} \approx \\ &\approx -\frac{3a^2}{2\pi} \left( \sqrt{1+b_C^2} + b_C \right) \log \frac{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C}{\Delta b_k}. \end{aligned} \quad (32)$$

It does not depend from magnon damping parameter.

## 4 The decoherence of two qubit entangled quantum states

The arbitrary state of pair spin-qubits in quantum register with zero Bloch vector values  $P(k, \tau) = 2 \text{Tr}_I I_k \rho_I(l, k, \tau) = P(l, \tau) = 0$  is described by the following reduced density matrix of nuclear spin system ( $\alpha, \beta = x, y, z$ ) (Ref.[5], §§2.5-2.7):

$$\rho_I(l, k, \tau) = \text{Tr}_{1, \dots, m \neq l, k, \dots, N} \rho_I(1, \dots, l, \dots, k, \dots, N, \tau) = 1/4 \left\{ 1 + \sum_{\alpha, \beta} 4G_{\alpha, \beta}(l, k, \tau) (I_{l, \alpha} \otimes I_{k, \beta}) \right\}. \quad (33)$$

The non-steady pair entanglement state will be determined in the form

$$\rho_I(l, k, \tau) = 1/4 \left\{ 1 + 4G_{z, z}(l, k, \tau) (I_{l, z} I_{k, z}) + G^{+, -}(l, k, \tau) (I_l^- I_k^+) + G^{-, +}(l, k, \tau) (I_l^+ I_k^-) \right\}, \quad (34)$$

where diagonal and non-diagonal elements of the matrix are defined as

$$G_{z, z}(l, k, \tau) = 4 \text{Tr} (I_{l, z} I_{k, z}) \rho_I(l, k, \tau), \quad (35)$$

$$G^{+, -}(l, k, \tau) = (G^{-, +}(l, k, \tau))^* = 4 \text{Tr} (I_l^+ I_k^-) \rho_I(l, k, \tau).$$

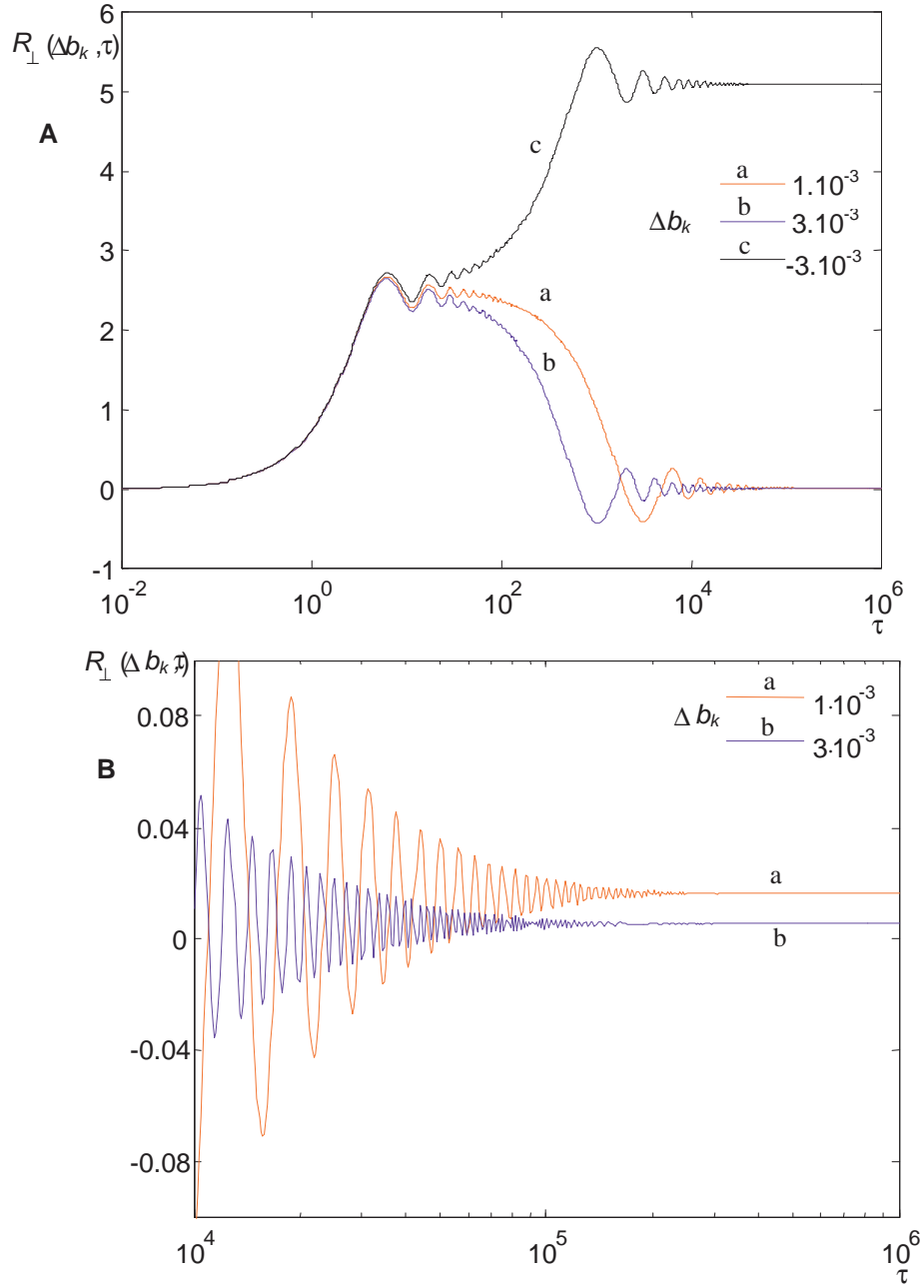


Figure 2: **A** The  $\tau$ -dependence of  $R_{\perp}(\Delta b_k, \tau)$  ( $\tau = t\omega_E$ ,  $\omega_E/2\pi \sim 10^{11}\text{Hz}$ ), for  $b_C^2 = 1/4$ ,  $s = 10^{-5}$  and  $\Delta b_k = b_C - b_k = -3 \cdot 10^{-3}, 1 \cdot 10^{-3}, 3 \cdot 10^{-3}$ . The case **B** corresponds to the enlarged values of  $R_{\perp}(\Delta b_k, \tau)$  only for  $\Delta b_k = 1 \cdot 10^{-3}, 3 \cdot 10^{-3}$  in the range of  $10^{-4} < \tau < 10^{-6}$ .



In the interaction representation relative Hamiltonian

$$h_0(l, k) = h_S - ((\omega_I(l) - a/2) I_z(l) + (\omega_I(k) - a/2) I_z(k)) \quad (36)$$

the reduced density matrix has the form

$$\rho_{in}(l, k, \tau) = \exp(ih_0(l, k)\tau) \rho(l, k, \tau) \exp(-ih_0(l, k)\tau). \quad (37)$$

Let there be the pure triplet entangled state of two removed spins  $l$  and  $k$  with zero total  $z$ -projection  $I = 1$ ,  $M = 0$ , which belongs to the same sublattice, realized by the certain external action in the initial moment  $\tau = 0$ . It will be described by reducer state vector  $|1, 0\rangle = \sqrt{1/2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$  or following density matrix:

$$\rho_I(l, k, 0) = |1, 0\rangle\langle 1, 0| = \frac{1}{2} \begin{vmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{vmatrix} = 1/4\{1 - 4(I_{l,z}I_{k,z}) + 2(I_l^- I_k^+) + 2(I_l^+ I_k^-)\}, \quad (38)$$

where  $G_{z,z}(l, k, 0) = -1$ ,  $G^{+, -}(l, k, 0) = G^{-, +}(l, k, 0) = 2$ . The concurrence of this entangled state has maximum value  $C = 1$ .

The evolution of such two-qubit state is due to the qubit interaction with magnons which in considered model is described by the following perturbation Hamiltonian in interaction representation

$$\Delta h_{IS}(l, k, \tau) = \Delta h_{IS}(l, \tau) + \Delta h_{IS}(k, \tau) = \quad (39)$$

$$= \exp(ih_0(l, k)\tau) (\Delta h_{IS}(l) + \Delta h_{IS}(k)) \exp(-ih_0(l, k)\tau),$$

where values  $\Delta h_{IS}(l, \tau)$ ,  $\Delta h_{IS}(k, \tau)$  are determined above by expression (8).

Let us suppose now (as previously in Sec.3), that the interaction of nuclear spins in ground coherent state (38) with electron system of the antiferromagnet is turning on at initial moment  $\tau = 0$  when non-disturbed density matrix has the form of direct product:  $\rho(0) = \rho_I(l, k, 0) \rho_S(0) = \rho_I(l, k, 0) |0\rangle\langle 0|$ .

We will write next the equation for density matrix in the interaction representation  $\rho_{in}(l, k, \tau)$ :

$$i\partial\rho_{in}(l, k, \tau) / \partial\tau = [\Delta h_{IS}(l, k, \tau), \rho_{in}(l, k, \tau)]. \quad (40)$$

From Eq.(40) for density matrix in the second theory of perturbation theory it is follow the equation

$$i\partial\rho_{in}(l, k, \tau) / \partial\tau = [\Delta h_{IS}(l, k, \tau), \rho_{in}(l, k, 0) |0\rangle\langle 0|] - \quad (41)$$

$$-i \int_0^\tau [\Delta h_{IS}(l, k, \tau), [\Delta h_{IS}(l, k, \tau'), \rho_I(l, k, 0) |0\rangle\langle 0|]] d\tau'.$$

By using Eq.(41) and making the cyclic permutation, we will obtain for the elements of reduced density matrix (34) the equations:

$$\partial(G_{z,z}(l, k, \tau)) / \partial\tau = 4 \text{Tr}_I (I_{l,z} I_{k,z}) \partial\rho_{in}(l, k, \tau) / \partial\tau \approx \quad (42)$$

$$\approx -4 \text{Tr}_I \int_0^\tau \langle 0 | [(I_{l,z} I_{k,z}), \Delta h_{IS}(l, k, \tau)], \Delta h_{IS}(l, k, \tau')] \rho_I(l, k, 0) |0\rangle d\tau',$$

and

$$\partial G^{+, -}(l, k, \tau) / \partial\tau = 4 \text{Tr} (I_l^+ I_k^-) \partial\rho_{in}(l, k, \tau) / \partial\tau \approx \quad (43)$$

$$\approx -4 \text{Tr} \int_0^\tau \langle 0 | [(I_l^+ I_k^-), \Delta h_{IS}(l, k, \tau)], \Delta h_{IS}(l, k, \tau')] \rho_I(l, k, 0) |0\rangle d\tau'.$$

Let us take into account Eq.(38), define the tensor longitudinal component in the form

$$G_{z,z}(l, k, \tau) = -\exp[-\gamma_{\parallel}(l, k, \tau)] \quad (44)$$

and the tensor transverse component in the form

$$G^{+,-}(l, k, \tau) = 2 \exp[i(\omega_I(l) - \omega_I(k))\tau - \gamma_{\perp}(l, k, \tau)]. \quad (45)$$

To obtain the expression for the rates of pair relaxation of longitudinal and transverse components in the context of second order of perturbation theory, we will write:

$$\partial G_{z,z}(l, k, \tau) / \partial \tau = d\gamma_{\parallel}(l, k, \tau) / d\tau = d\gamma_{\parallel}^*(l, k, \tau) / d\tau = \quad (46)$$

$$\begin{aligned} &= -4 \text{Tr}_I \int_0^{\tau} \langle 0 | [(I_{l,z} I_{k,z}), \Delta h_{IS}(l, k, \tau), \Delta h_{IS}(l, k, \tau')] (-I_{l,z} I_{k,z} + 1/2 (I_l^+ I_k^-) + 1/2 (I_l^- I_k^+)) | 0 \rangle d\tau' = \\ &= d\gamma_{\parallel}(l, \tau) / d\tau + d\gamma_{\parallel}(k, \tau) / d\tau + d\tilde{\Gamma}_{\parallel}(k, l - k, \tau) / d\tau \end{aligned}$$

and

$$\text{Re } \partial G^{+,-}(l, k, \tau) / \partial \tau = -2 \text{Re } d\gamma_{\perp}(l, k, \tau) / d\tau = \quad (47)$$

$$\begin{aligned} &= -4 \text{Re Tr}_I \int_0^{\tau} \langle 0 | [(I_l^+ I_k^-), \Delta h_{IS}(l, k, \tau), \Delta h_{IS}(l, k, \tau')] (-I_{l,z} I_{k,z} + 1/2 (I_l^+ I_k^-) + 1/2 (I_l^- I_k^+)) | 0 \rangle d\tau' = \\ &= -2 \text{Re } d\gamma_{\perp}(l, \tau) / d\tau - 2 \text{Re } d\gamma_{\perp}(k, \tau) / d\tau - 2 \text{Re } d\tilde{\Gamma}_{\perp}(k, l - k, \tau) / d\tau, \end{aligned}$$

where the correlation part of longitudinal two spin relaxation rate

$$\begin{aligned} &d\tilde{\Gamma}_{\parallel}(k, l - k, \tau) / d\tau = \\ &= -4 \text{Tr}_I \int_0^{\tau} \langle 0 | [I_{l,z}, \Delta h_{IS}(l, \tau)] I_{k,z}, \Delta h_{IS}(k, \tau')] ((I_l^+ I_k^-) + (I_l^- I_k^+)) | 0 \rangle d\tau' = \\ &= -\frac{a^2}{4} 4 \text{Re} \int_0^{\tau} \langle 0 | [S_k^+(\tau'), S_l^-(\tau)] | 0 \rangle d\tau'. \end{aligned} \quad (48)$$

Consider next the correlation part of transverse two spin decoherence rate

$$\begin{aligned} &\text{Re } d\tilde{\Gamma}_{\perp}(k, l - k, \tau) / d\tau = \\ &= -2 \text{Re Tr}_I \int_0^{\tau} \langle 0 | [I_l^+, \Delta h_{IS}(l, \tau)] I_k^-, \Delta h_{IS}(k, \tau')] (I_{l,z} I_{k,z}) + \\ &\quad + [I_k^-, \Delta h_{IS}(k, \tau)] I_l^+, \Delta h_{IS}(l, \tau')] (I_{l,z} I_{k,z}) | 0 \rangle d\tau' = \\ &= -\frac{a^2}{4} 2 \text{Re} \int_0^{\tau} \langle 0 | [S_k^-(\tau'), S_l^+(\tau)] + [S_k^+(\tau'), S_l^-(\tau)] | 0 \rangle d\tau' = \\ &= -\frac{a^2}{4} 4 \text{Re} \int_0^{\tau} \langle 0 | [S_k^+(\tau'), S_l^-(\tau)] | 0 \rangle d\tau', \end{aligned} \quad (49)$$

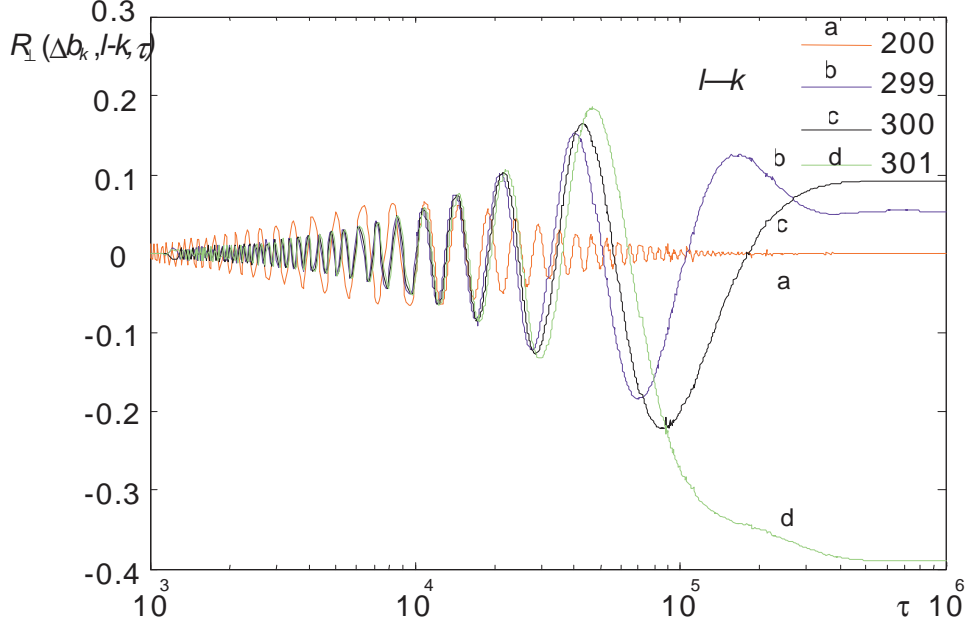


Figure 3: The  $\tau$ -dependence of decoherence rate  $R_{\perp}(\Delta b_k, l-k, \tau)$  for values  $\Delta b_k = 3.10^{-3}$ ,  $s = 10^{-5}$ ,  $l-k = 200, 299, 300, 301$ .

that is the correlation part of decoherence rate is equal to the correlation part of longitudinal relaxation rate.

Let us rewrite next the expression (49) similarly as it would made in Sec.3, accounting only low magnon excitation mode with energy  $E_-$ :

$$\begin{aligned}
& \text{Re } d\tilde{\Gamma}_{\perp}(k, l-k, \tau) / d\tau \approx \\
& \approx \frac{a^2}{(4\pi)^2} 2 \text{Re} \int_0^{\tau} \int_0^{\tau} u^*(q_{\perp}, E) u(q'_x, q_y, E) \exp(-i(E_- - s)(\tau' - \tau)) \exp[i(q_x k - q'_x l)] dE dq_{\perp} dq'_x d\tau' = \\
& = \frac{a^2}{(4\pi)^2} \int \frac{\sqrt{1+b_C^2} + E(q_{\perp})}{E(q_{\perp})} \cdot \left\{ \frac{-(E(q_{\perp}) - b_{(l+k)/2}) \sin(q_x(l-k)) + s \cos(q_x(l-k))}{(E(q_{\perp}) - b_{(l+k)/2})^2 + s^2} + \right. \\
& \left. + \frac{[(E(q_{\perp}) - b_{(l+k)/2}) \sin((E(q_{\perp}) - b_{(l+k)/2})\tau - q_x(l-k)) - s \cos((E(q_{\perp}) - b_{(l+k)/2})\tau - q_x(l-k))] \exp(-s\tau)}{(E(q_{\perp}) - b_{(l+k)/2})^2 + s^2} \right\} dq_{\perp}.
\end{aligned} \tag{50}$$

Taking next in to account that  $\int_0^{2\pi} \sin[q_{\perp} \cos \varphi (l-k)] d\varphi = 0$  and introducing again the variable  $\xi = E(q_{\perp}) - b_C$ , we will write  $E(q_{\perp}) - b_{(l+k)/2} = E(q_{\perp}) - b_k - g(l-k)/2 = \xi + \Delta b_k - g(l-k)/2$  and obtain (Fig. 3)

$$\begin{aligned}
& \frac{2\pi}{3a^2} \text{Re } d\tilde{\Gamma}_{\perp}(k, l-k, \tau) / d\tau \approx R_{\perp}(\Delta b_k, l-k, \tau) = \\
& = \int_0^{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C} \left( \sqrt{1+b_C^2} + b_C + \xi \right) Y(\xi + \Delta b_k - g(l-k)/2, \tau) J_0 \left( \sqrt{12[(b_C + \xi)^2 - b_C^2]} (l-k) \right) d\xi.
\end{aligned} \tag{51}$$

The decoherence rates of entangled qubit pair are due to decoherence of one spin states  $l, k$  and also to the correlation between nuclear spins  $l, k$ . The initial diagonal and non-diagonal elements of density matrix  $1 + G_{z,z}(l, k, \tau)$  and  $G^{+, -}(l, k, \tau)$  are decreased with full rates  $\text{Re } d\Gamma_{\parallel}(l, k, \tau) / d\tau$  and  $\text{Re } d\Gamma_{\perp}(l, k, \tau) / d\tau$ . Note

that the asymptotic value for correlation part of decoherence rate (Fig. 3) may periodically change sign, if  $\Delta b_k - g(l-k)/2 < 0$ , that is for states after ‘‘turning point’’. Likewise, the indirect interspin interaction is described by precisely the same oscillating sign-changing function after ‘‘turning point’’ (see Eq. (74) in Ref.[4]).

The concurrence for entangled two-qubit state can be obtained by using the Wootters formula (Ref.[6])

$$C(l, k, \tau) = 1/2 \max\{|G^{+, -}(l, k, \tau)| - (1 + G_{z,z}(l, k, \tau)); 0\}. \quad (52)$$

Taking in to account that  $\text{Re } \gamma_{\perp}(k, \tau) = \gamma_{\parallel}(k, \tau)$ ,  $|G^{+, -}(l, k, \tau)| \approx 2 \exp(-\text{Re } \gamma_{\perp}(l, k, \tau))$ ,  $G_{z,z}(l, k, \tau) \approx -\exp(-\gamma_{\parallel}(l, k, \tau))$  and also Eqs (44), (45), (47), we will obtain

$$C(l, k, \tau) = 1/2 \{3 \exp(-\text{Re } \gamma_{\perp}(l, \tau) - \text{Re } \gamma_{\perp}(k, \tau) - \text{Re } \tilde{\Gamma}_{\perp}(k, l-k, \tau)) - 1\}. \quad (53)$$

For the concurrence-damping rate we will then write

$$\begin{aligned} dC(l, k, \tau)/d\tau &= -3/2d \left( \text{Re } \gamma_{\perp}(l, \tau) + \text{Re } \gamma_{\perp}(k, \tau) + \text{Re } \tilde{\Gamma}_{\perp}(k, l-k, \tau) \right) d\tau = \\ &= -\frac{9a^2}{2\pi} (R_{\perp}(\Delta b_l, \tau) + R_{\perp}(\Delta b_k, \tau) + R_{\perp}(\Delta b_k, l-k, \tau)). \end{aligned} \quad (54)$$

Note, that for  $\Delta b_k > 0$  parameter  $\Delta b_l = \Delta b_k - g(l-k)$  can change the sign. The expression  $R_{\perp}(\Delta b_l, \tau)$  takes the form

$$R_{\perp}(\Delta b_l, \tau) = R_{\perp}(\Delta b_k - g(l-k), \tau) = \int_0^{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C} \left( \sqrt{1 + b_C^2} + b_C + \xi \right) Y(\xi + \Delta b_k - g(l-k), \tau) d\xi \quad (55)$$

Finally, for the value of concurrence damping rate we will obtain

$$dC(l, k, \tau)/d\tau = -\frac{9a^2}{2\pi} R_{\perp}^{\Sigma}(\Delta b_k, l-k, \tau), \quad (56)$$

where (Fig. 4)

$$\begin{aligned} R_{\perp}^{\Sigma}(\Delta b_k, l-k, \tau) &= R_{\perp}(\Delta b_k, \tau) + R_{\perp}(\Delta b_l, \tau) + R_{\perp}(\Delta b_k, l-k, \tau) = \\ &= \int_0^{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C} \left( \sqrt{1 + b_C^2} + b_C + \xi \right) \cdot [Y(\xi + \Delta b_k, \tau) + Y(\xi + \Delta b_k - g(l-k), \tau) + \\ &+ Y(\xi + \Delta b_k - g(l-k)/2, \tau) J_0 \left( \sqrt{12 [(b_C + \xi)^2 - b_C^2]} (l-k) \right)] d\xi. \end{aligned} \quad (57)$$

The concurrence damping rate tends at  $\tau \rightarrow \infty$  to positive value:

$$\begin{aligned} R_{\perp}^{\Sigma}(\Delta b_k, l-k, \infty) &= s \int_0^{\sqrt{b_C^2 + \frac{\pi^2}{12}} - b_C} \left( \sqrt{1 + b_C^2} + b_C + \xi \right) \left[ \frac{1}{(\xi + \Delta b_k)^2} + \frac{1}{(\xi + \Delta b_k - g(l-k))^2} + \right. \\ &\left. + \frac{J_0 \left( \sqrt{12 [(b_C + \xi)^2 - b_C^2]} (l-k) \right)}{(\xi + \Delta b_k - g(l-k)/2)^2} \right] d\xi > 0. \end{aligned} \quad (58)$$

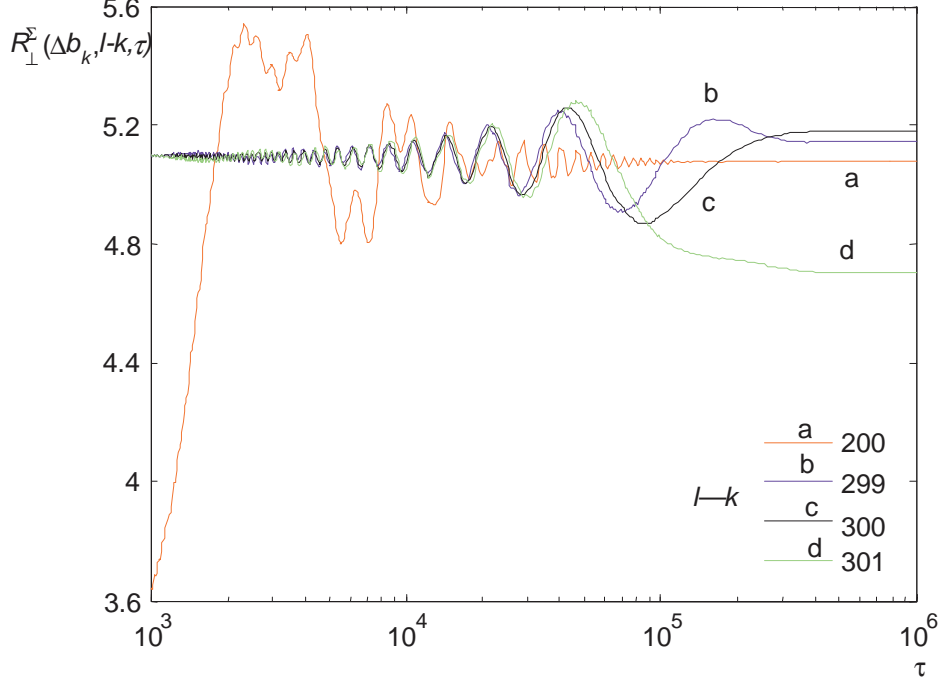


Figure 4: The  $\tau$ -dependence of  $R_{\perp}^{\Sigma}(\Delta b_k, l-k, \tau)$  for values  $\Delta b_k = 3.10^{-3}$ ,  $s = 10^{-5}$ ,  $l-k = 200, 299, 300, 301$ .

## 5 Adiabatic decoherence caused by interaction with nuclear spins of random distributed isotopes substituting the basic isotopes in antiferromagnetic structure.

Between other mechanisms of decoherence it should be pointed out the adiabatic mechanism that is determined by magnetic interaction of nuclear spins-qubits with electron and nuclear spins of impurity atoms, which play here role of an environment (Ref.[5], §5.4).

Interaction of nuclear spins with magnetic moments of impurity paramagnetic atoms is of no concern as compared to the interaction of nuclear spins with electron spins of own atoms. This mechanism is largely suppressed for a high degree of electron spin polarization (at  $B/T > 30$  T/K).

Let us consider here a decoherence model, where nuclear spin-qubit interact with nuclear magnetic moments of randomly distributed impurity isotopes in basic nuclear spin-free antiferromagnet.

Hamiltonian of dipole-dipole magnetic interaction of considered nuclear spins has the following form:

$$H_{I,I_{imp}} = \hbar \sum_{i,\alpha\beta}^N D_{\alpha\beta}(r_i) I_{\alpha} I_{\beta,imp}(r_i, t), \quad (59)$$

where

$$D_{\alpha\beta}(r_i) \frac{\mu_0 \gamma_I \gamma_{I,imp} \hbar}{4\pi r_i^3} \left( \delta_{\alpha\beta} - \frac{3r_{i\alpha} r_{i\beta}}{r_i^2} \right), \quad (60)$$

$\gamma_I/2\pi$ ,  $\gamma_{I,imp}/2\pi$  are giromagnetic ratio of quantum register nuclear spin-qubit and of impurity isotope nuclear spin,  $\mathbf{r}_i$  is radius-vector of distance from the position of nuclear spin-qubit to position of  $i$ -th impurity nuclear spin,  $\gamma_{I,imp} \hbar I_{\beta,imp}(r_i, t)$  is fluctuating magnetic moment of impurity isotope, which produce the random local field:

$$\Delta B_{\alpha}(t) = - \sum_{i,\beta}^N D_{\alpha\beta}(r_i) (I_{\beta,imp}(r_i, t) - \langle I_{\beta,imp}(r_i) \rangle) / \gamma_I. \quad (61)$$

The mean value  $\langle \gamma_I B_\alpha(t) \rangle = \sum_{i,\beta}^N D_{\alpha\beta}(r_i) \langle I_{\beta,imp}(r_i) \rangle$  determines the shift of qubit resonance frequency.

The correlation function for random modulation of nuclear spin resonance frequency is determined by the following expression

$$\langle \Delta\omega(\tau) \Delta\omega(0) \rangle = C_{I,imp} \int \sum_{\beta} D_{z\beta}^2(r) (\langle I_{\beta,imp}(r,\tau) I_{\beta,imp}(r,0) \rangle - \langle I_{\beta,imp}(r) \rangle^2) dr, \quad (62)$$

where  $C_{I,imp}$  is concentration of impurity isotopes .

The expression for correlation function in considered case of adiabatic decoherence takes the form

$$\langle \Delta\omega(\tau) \Delta\omega(0) \rangle = \langle \Delta\omega^2 \rangle \exp(-t/T_{||,imp}), \quad (63)$$

where quadratic mean value of modulation frequency

$$\langle \Delta\omega^2 \rangle = C_{I,imp} \left( \frac{\mu_0}{4\pi} \gamma_I \gamma_{I,imp} \hbar \right)^2 \frac{16\pi}{15a^3} (\langle I_{z,imp}^2 \rangle - \langle I_{z,imp} \rangle^2), \quad (64)$$

$$\langle I_{z,imp}^2 \rangle - \langle I_{z,imp} \rangle^2 = (1 - \tanh^2(\gamma_{I,imp} B \hbar / 2kT_I)) / 4, \quad (65)$$

$a$  is minimal distance to impurity nuclear spin, with is of order of lattice constant  $\sim 1$  nm.

If it is believed that  $T_{||,imp} \sim 10^4$  sec  $\gg T_D$  (the so-called condition of rigid lattice) and that  $T_D > 1$  sec, for the determination of allowable isotope concentration we will obtain the condition

$$1/T_D^2 \approx \langle \Delta\omega^2 \rangle = C_{I,imp} \left( \frac{\mu_0}{4\pi} \gamma_I \gamma_{I,imp} \hbar \right)^2 \frac{4\pi}{15a^3} (1 - \tanh^2(|\gamma_{I,imp}| B \hbar / 2kT_I)) < 1 \text{ sec}^{-2}. \quad (66)$$

For values  $B/T > 30$  T/K we will obtain for allowable concentration of impurity isotopes the highly rigid condition  $C_{I,imp} < 10^{15} \text{ cm}^{-3}$ , ( $\sim 10^{-5}$  %). However, if temperature  $T_I$  for nuclear spins of impurity isotopes corresponds to value, for which almost full nuclear spin polarization takes place  $|\gamma_{I,imp}| B \hbar / kT_I > 1$ , that is  $T_I < 1$  mK, so the allowable concentration in isotope-pure antiferromagnet will  $C_{I,imp} \% < 4.5 \cdot 10^{-2} \%$ . It will rapidly increase on further lowering of nuclear spin temperature.

Eventually the suppressing of this mechanism calls for appropriate cleaning of substrate from impurity atoms and using very low spin temperatures for nuclear spins.

## 6 The encoded DFS (Decoherence-Free Subspaces) logical qubits are constructed on clusters of the four-physical qubits

Let us consider here two encoded DFS logical qubits  $|0_L\rangle$  and  $|1_L\rangle$  with zero total angular momentum  $J = 0$ ,  $m_J = 0$ , which states are constructed on cluster of four states of physical qubits:

$$|0_L\rangle = 1/2 [(|01\rangle - |10\rangle) \otimes (|01\rangle - |10\rangle)] \quad (67)$$

$$|1_L\rangle = 1/\sqrt{3} [|11\rangle \otimes |00\rangle + |00\rangle \otimes |11\rangle - 1/2 (|01\rangle + |10\rangle) \otimes (|01\rangle + |10\rangle)].$$

They form two dimensional subspace for quantum operation.

As is shown in Refs. [7-9] this subspace represent, as it is called, the strong collective decoherence free subspace (DFS), if the states of four physical qubits are the eigenstates of Hamiltonian with antiferromagnetic interaction ( $\Delta > 0$ ) of XXX type in the absent of external field

$$h_{xxx}^4 = \Delta/2 \sum_{k \neq l}^4 I(k) I(l) = \Delta/2 \left\{ \sum_k^4 I(k) \sum_l^4 I(l) - \mathbf{31} \right\}, \quad (68)$$

where  $\mathbf{1}$  is unit four-dimensional matrix (here symbol  $\otimes$  is omitted) and is not relevant. It has eigenvalues  $\Delta/2 J(J+1)$  with  $J = 0, 1, 2$  The DFS states (67) are the lowest state which identical to ground state of Hamiltonian (68) with  $J = 0$ ,  $m = 0$  and has two-fold degeneracy.

We will use now the before obtained expression for effective Hamiltonian of two nuclear spins, belonging to common sublattice in quantum register ([4], Eq.(A2.8)) with interaction of XX0 or two-dimensional isotropic type:

$$h_{xxo} = - \sum_{j=k,l} \{[\omega_I(j) - a/2 - W(j)] I_z(j) + U(j,j)/2 - U(k,l) [I^-(k) I^+(l) + I^+(k) I^-(l)]\} \quad (69)$$

We write next the total nuclear spin Hamiltonian of quantum register neglecting the terms  $W(j) \approx U(j,j) = \text{Const.}$  of order of  $a^2$  and take in to account that the difference of  $\omega_I(k) - \omega_I(l) = \gamma_I/\gamma_S g(k-l) \ll a \sim 10^{-3}$  for  $(k-l) < 1/g \sim 10^5$ :

$$h_{II} = -(\omega_I - a/2) \sum_k I_z(k) - \sum_{k \neq l} U(k,l) [I^-(k) I^+(l) + I^+(k) I^-(l)]. \quad (70)$$

Our Hamiltonian (70), written for four qubits, differs from Eq.(68) in that it has identical values of interaction parameter  $\Delta$  for different qubit pairs and it is free from the term  $\sum_{k \neq l}^4 I_z(k) I_z(l)$ . In addition, the Hamiltonian (70) has operator  $\sum_k I_z(k)$ .

In Ref.[4] it was obtained that the dependence of indirect interspin interaction  $U(k,l)$  from distance for  $(l-k) > 2\Delta b_k/g = 2(b_C - b - gk)/g$  takes oscillating character with quasi-period which gradually decreased with increasing of the distant  $(l-k)$ . In this case indirect interaction periodically change the sign. Consequently, it is possible to choose the nuclear spin position in such a way that the value of interaction  $U(k,l) = -U < 0$  would be the same for all four qubit position in the nuclear spin chain considered as a quantum register.

$$\begin{aligned} h_{xxo}^4 &= -(\omega_I - a/2) \sum_{k=0}^4 I_z(k) + U \{1/2 \left[ \sum_{k=0}^4 I^-(k) \sum_{l=0}^4 I^+(l) + \sum_{k=0}^4 I^+(k) \sum_{l=0}^4 I^-(l) \right] - 2\mathbf{1}\} = \\ &= -(\omega_I - a/2) \sum_{k=0}^4 I_z(k) + U \{ \sum_{k=0}^4 I(k) \sum_{l=0}^4 I(l) - \sum_{k=0}^4 I_z(k) \sum_{l=0}^4 I_z(l) - 2\mathbf{1} \} \end{aligned} \quad (71)$$

The identity component of  $h_{xxo}^4$  in Eq.(71) is not relevant here and will be next omitted. The eigenvalues of such Hamiltonian are

$$E(J, m_J) = -|\omega_I - a/2| m_J + U (J(J+1) - m_J^2), \quad m_J = 0, \pm 1, \dots, \pm J, \quad J = 0, 1, 2. \quad (72)$$

They are tabulated below in Table:

	$J = 0$	$J = 1$	$J = 2$
$m_J = 0$	0	$2U$	$6U$
$m_J = \pm 1$		$\pm \omega_I - a/2  + U$	$\pm \omega_I - a/2  + 5U$
$m_J = \pm 2$			$2\pm \omega_I - a/2  + 2U$

Because that  $|\omega_I - a/2| \gg U \sim a^2$ , the states of four considered physical qubits here represent approximate so-named weak collective decoherence free subspace (Ref.[9]). The ground state of Hamiltonian (71) corresponds to nondegenerate state with  $J = 2, m_J = -2$  and to eigenvalue  $-2|\omega_I - a/2| + 2U$ . It can not use for two logical qubit encoding.

However the all states with  $m_J = 0$  are identical to the strong collective DFS state with  $J = 0, m_J = 0$  which overlie the ground state by  $2|\omega_I - a/2| - 2U$ . It is represented by two-fold degenerated state of Eq.(67) type. This state at low temperatures  $|\omega_I - a/2| \gg T/(\hbar\omega_E/k_B)$  ( $T \sim 1$  mK) is a metastable state and, consequently, can be used as two DFS encoded logical qubits.

## Conclusion

It was considered the results of theoretical investigations of one qubit and two qubit nonadiabatic decoherence and longitudinal relaxation caused by interaction of nuclear spins-qubits with virtual magnon excitations in antiferromagnet. It turns out that the character of decoherence processes essentially depends on antiferromagnet anisotropy (parameter  $b_C$ ) and on inhomogeneity of external field (parameter  $g$ ). As this takes place, the temperature whereby the thermal magnon excitations are excluded and the two-magnon spin-lattice relaxation is especially suppressed, should be defined by values  $T \ll T_C (1 - b/b_C)$ ,  $T_C = \hbar\gamma_S B_C/k_B$ . As an example we have also considered decoherence of pair qubits maximally entanglement state and have calculated the concurrence damping rate.

The other mechanism of quantum state decoherence is adiabatic process of the resonance nuclear spin frequency modulation caused by dipole-dipole interaction with nuclear spins of impurity isotopes. The necessary degree of the adiabatic decoherence suppression can be obtained at spin temperature less than 1mK and for the concentration of impurity nuclear spin containing isotopes less than  $10^{-2}\%$ .

Finally it was discussed for considered model of quantum register the possibility of construction of DFS-states.

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