The controlled indirect coupling between spatially-separated qubits in antiferromagnet-based NMR quantum registers

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ABSTRACT

It is considered the indirect inter-qubit coupling in 1D chain of atoms with nuclear spins 1/2, which plays role of qubits in the quantum register. This chain of the atoms is placed by regular way in easy-axis 3D antiferromagnetic thin plate substrate, which is cleaned from the other nuclear spin containing isotopes. It is shown that the range of indirect inter-spin coupling may run to a great number of lattice constants both near critical point of quantum phase transition in antiferromagnet of spin-flop type (control parameter is external magnetic field) and/or near homogeneous antiferromagnetic resonance (control parameter is microwave frequency).

Keywords: Qubit, quantum register, nuclear spin, indirect nuclear spin coupling and easy-axis antiferromagnet

1. INTRODUCTION

In 1998 B.Kane proposed the scheme of large-scale NMR quantum register, based on nuclear spin-free substrate $^{28}$Si, into a near-surface layer of which atoms $^{31}$P, whose nuclear spins 1/2 play the role of qubits, are implanted in the form of a regular chain. One of the main quantum operations is a two-qubit operation, such as CNOT-operation, for which it is needed to switch on a coupling between considered qubits. It is assumed, that the indirect nuclear spin coupling for neighboring donors is controlled by special gates and two-qubit operations for far spatially separated qubits can be produced using SWAP operations between neighboring qubits. The separation between neighboring donors in this scheme must be $\sim 20$ nm. A model of NMR quantum register based on two-leg ladder 1D antiferromagnet chain, where nuclear spins-qubits are placed in the magnetic field gradient and separated by a distance up to several tens of lattice constants, was proposed in [2]. The needed indirect inter-qubit coupling of Shul-Nakamura type in this model must be switched on by the external magnon packet excitations in the antiferromagnetic chain. Authors of^2 assume some organic materials as the possible candidates for the NMR quantum register base.

In this paper, we consider a model of NMR quantum register, which is based on the easy-axis 3D antiferromagnet at low temperature. It is shown that the range of indirect coupling can range up to a great number of lattice parameters both near critical point of quantum phase transition in antiferromagnet of spin-flop type and/or near homogeneous antiferromagnetic resonance.

2. EASY-EXIS ANTIFERROMAGNETS FOR NMR QUANTUM REGISTERS

We propose here that 1D chain of atoms with nuclear spins is placed in easy-axis 3D antiferromagnetic thin substrate-plate ($d$ is the thickness), which is cleaned from the other nuclear spin containing isotopes (Fig. 1).

Consider next a symmetric easy-axis antiferromagnetic structure (rhomboedric, trigonal or hexagonal crystal symmetry). The qubits with numbers $i$ and $j$ are separated by distance $x_{ij} \equiv a(i-j)$ ($a$ is lattice parameter) along the plate. As examples, the following well-known easy-axis natural crystals FeCO$_3$ (siderite), Fe$_2$O$_3$(hematite), CeCu$_2$, FeGe, FeGe$_2$ may be probably proposed. The isotopes $^{13}$C, $^{57}$Fe are here as nuclear spin containing atoms when they substitute for the definite host spin-free atoms in plate. The indirect inter-qubit coupling is due to hyperfine interaction of nuclear and electron spins in substituted atom, coupling of that electron spin is mainly through exchange interactions with electron spin of the neighboring host atom and spin-wave (magnon) propagation that is caused by the exchange interaction between electron spins of host atoms. The external homogenous field $B$ (z-axis) is directed normally to the surface of plate and in parallel with the easy-axis.
Figure 1. The scheme of antiferromagnet based NMR quantum register. The nuclear spin is contained only in atoms A.

Let us use for an antiferromagnet model the system of two magnetic sublattices A and B with \( \frac{L}{2} \) sites in each sublattice (\( L \) is even full site number). The sites will be numbered by numbers \( i \) and \( j \) accordingly.

The electron spin Hamiltonian for our model for 3D easy-axis antiferromagnets with interaction only between neighboring atoms may be represented as (in frequency units)

\[
H_S = \gamma_S B \left( \sum_{i}^{\frac{L}{2}} S_Az(i) + \sum_{j}^{\frac{L}{2}} S_Bz(j) \right) +
+ \frac{2\gamma_S}{Z} \sum_{\delta}^{\frac{Z}{2}} \{ B_E S_A(i) S_B(i + \delta) + B_A S_Az(i) S_Bz(i + \delta) \},
\]

where \( S_A \) and \( S_B \) are electron spin operators, \( Z \) is the number of neighboring atoms, \( B_E > B_A \geq 0 \) are exchange and anisotropy fields for easy-axis antiferromagnet, \( \gamma_S = 176.08 \, \text{GHz/T} \) is gyromagnetic ratio for electron spin.

Under low temperature conditions, the electron spins are essentially in ground state and deviations of their states from ground state are small and may be considered in spin-wave approximation.

Spin-wave (magnon) Hamiltonian after diagonalization, as it is known, takes the form

\[
H_S \approx \text{Const} + \sum_{\mathbf{k}} (\omega_{+}(\mathbf{k}, B) N_{+}(\mathbf{k}) + \omega_{-}(\mathbf{k}, B) N_{-}(\mathbf{k}),
\]

where \( \omega_{\pm}(\mathbf{k}, B) \) are long-wave magnon frequencies (\( k_\perp a_\perp, k_z a_z \ll 1 \)), where \( k_\perp \) is radial component, are

\[
\omega_{\pm}(k, B) \approx \gamma_S \left( \sqrt{\xi^2 B_E^2 (a_{\perp}^2 k_\perp^2 + a_z^2 k_z^2) + 2B_A B_E + B_A^2 \pm B} \right),
\]

where \( \xi^2 \sim 1 \), \( a_\perp \) and \( a_z \) are lattice parameters of the order of lattice constants.

We see that magnon spectrum of easy-axis antiferromagnetic has energy gap

\[
\omega_{-}(0, B) > 0
\]

for fields \( B < B_C = \sqrt{2B_A B_E + B_A^2} \), where value of \( B_C \) is in the neighborhood of 10 tesla.

Under low temperature condition (\( k_B \) is Boltzmann constant)

\[
T \ll \hbar \omega_{-}(0, B) / k_B = T_C (1 - B/B_C),
\]
where \( T_C = \hbar \gamma_S B_C / k_B \) is less than 10 K, the easy-axis antiferromagnet conserves homogeneous ground state. This condition provides also a very long transverse nuclear spin relaxation time \(^4\) and accordingly the one qubit decoherence time.

If the field \( B \) (control parameter) goes through the critical field \( B_C \), the stability of grand state breaks down (Goldstone instability) and the quantum phase transition in the homogeneous \((k = 0)\) spin-flop phase occurs.

Let us move now to condition of antiferromagnetic resonance. In the presence of the rotating transverse microwave field with frequency \( \omega \) (control parameter), the \( B \) is replaced by

\[
B \rightarrow B_{\text{eff}}(\omega) = (B + \omega / \gamma_S).
\]

The lower magnon frequency in rotating frame takes now the form

\[
\omega_(k, B, \omega) \approx \gamma_S \left( \sqrt{\xi^2 B_E^2 (a_\perp^2 k_\perp^2 + a_z^2 k_z^2) + B_C^2 - B_{\text{eff}}(\omega)} \right).
\]

The homogeneous \((k = 0)\) antiferromagnetic resonance corresponds to phase transition due to instability in rotating frame:

\[
\omega_(0, B, \omega) = 0, \text{or} \omega = \gamma_S (B_C - B).
\]

Let us assume that antiferromagnetic resonance width obeys the conditions \( \Delta \omega < \gamma_S B_C \ll \omega_0 = \gamma_S \xi^2 B_E^2 / B_C \) and thickness \( d \) of infinitely large plate is \( d < \pi a_z (\omega_0 / \Delta \omega_0)^{1/2} \), that is, in neighbourhood of nanometers. Then the 2D (along the plate surface, \( k_\perp \neq 0, k_z = 0 \)) spin waves are defined as homogeneous electron spin precession normally to the plate surface or as zero mode of spin-wave (magnon) resonance.

\[
\omega_(k_\perp, k_z = 0, B, \omega) = 0,
\]

and we have the value for microwave frequency

\[
\omega \approx \gamma_S \left( \sqrt{\xi^2 B_E^2 a_\perp^2 k_\perp^2 + B_C^2} - B \right).
\]

For homogeneous microwave field and for large plate wave vector \( k_\perp \) take the continuous values \( 0 \leq k_\perp < \infty \), therewith value \( k_\perp = 0 \) corresponds to homogeneous antiferromagnetic resonance in 2D structure (thin plate).

### 3. CONTROLLED INDIRECT INTER-QUBIT COUPLING IN EASY-AXIS ANTIFERROMAGNET

The indirect inter-spin coupling in chain is due to hyperfine interaction of nuclear and electron spins in substituted atoms \( A \) in chain \( A(I_A S_A) \), where \( A \) is isotropic hyperfine coupling constant of the order of 100 MHz. Electron spins of the neighboring host atom \( A \) and \( B \) are coupled mainly through the exchange interactions, which is responsible for 2D spin waves (magnons) formation in particular with the frequency \( \omega_(k, B) \). The nuclear spin of an atom \( A \) exits the magnon, which is absorbed by nuclear spin of another atom \( A \) (or \( B \)). In this way, the coupling between nuclear spins of separated atoms is produced. Note that no external spin wave excitation is involved here.
We restrict our consideration to the indirect inter-nuclear interaction at low temperature. The corresponding Shul-Nakamura Hamiltonian for two spins in one sublattice A i and j are located along x-axis is nonzero only for transverse component:

\[ H_I = -I_{\perp}(i - j) \left( I_{Ax}(i)I_{Ax}(j) + I_{Ay}(i)I_{Ay}(j) \right) - \gamma_S B \ (I_{Az}(i) + I_{Az}(j)) \],

where value of indirect nuclear inter-spin coupling have form

\[ I_{\perp}(i - j) = \frac{A^2}{2N} \sum_k \exp(k_{\perp}a_{\perp}(i - j) \cos \varphi) / \omega (k_{\perp}, k_z = 0, B, \omega), \]

where N is the full number of atoms in the plate. The function (11) represents essentially a correlation function for transverse components of electron spin operators.

We assume next that for large value of distance |i - j| the dominant contribution gives small values of radial spin vectors \( k_{\perp}a_{\perp} < (BC/E) \ll 1 \). Then we are coming from summation to integration over polar angle \( \varphi \) and \( k_{\perp} \) and obtain

\[
I_{\perp}(i - j) \approx \frac{A^2a_z^2}{(\gamma_S4\pi d)} \int_0^\infty J_0(k_{\perp}a_{\perp}(i - j) / \omega ) / (BC - B_{\text{eff}}(\omega) + \xi^2B_E^2a_z^2k_{\perp}^2/2BC) \ k_{\perp}dk_{\perp} = \]
\[
= \frac{A^2a_z}{(\gamma_S4\pi d)} \int_0^\infty J_0(\zeta (i - j)) / (BC - B_{\text{eff}}(\omega) + \xi^2B_E^2\zeta^2/2BC) \ \zeta \ d\zeta, \]

where \( J_0(x) \) is the Bessel function.

We now obtain

\[ I_{\perp}(i - j) \approx \frac{A^2a_z}{BC} B_C / (\gamma_S2\pi dB_E^2) \cdot K_0(||i - j||/\rho_B(\omega)), \]

where \( K_0(x) \) is McDonald function and for \( B_{\text{eff}}(\omega) \leq B_C \)

\[ \rho_B(\omega) = \rho_0 / (1 - B_{\text{eff}}(\omega) / B_C)^{1/2}, \]

denotes the controlled range of indirect nuclear spin coupling (correlation length), \( \rho_0 = \xi B_E / \sqrt{2}B_C \) may be of the order of ten.

Let us consider two simple cases:

a) Away from the point of phase transition and antiferromagnetic resonance \( B_{\text{eff}}(\omega) / B_C \ll 1 \), \( \rho_B(\omega) = \rho_0 \) we obtain

\[ (2\pi d^2 \gamma_S B_E^2 / A^2a_z B_C) \cdot I_{\perp}(i - j) \approx (\pi \rho_0 / 2|i - j|)^{1/2} \exp(-|i - j|/\rho_0) \ll 1 \]

The indirect inter-spin coupling is relatively weak for any one \(|i - j| \geq 10\rho_0\).

b) Both near electron quantum phase transition (\( \omega = 0 \)) and near antiferromagnetic resonance (\( \omega \neq 0 \) for \( (1 - B_{\text{eff}}(\omega)) / B_C \ll 1 \) we have
\[ \rho_0 \ll \rho_B(\omega); \ |i-j|/\rho_B(\omega) \ll 1 : \]  

and

\[ (2\pi d^2 \gamma_S B_E^2 /A^2 a_z B_C) \cdot I_4 (i-j) \approx \log \left(2\rho_B(\omega)/|i-j|\right) \gg 1. \]  

We see that increase of correlation length is attended with a decrease of energy gap. However, the temperature therewith must correspond to low values \( T \ll T_C (1-B_{\text{eff}}(\omega)/B_C) \). As a result, the controlled indirect coupling may be large for distances \( |i-j| \) as much as great number of lattice parameters.

4. CONCLUSION

We have shown that there is possibility to control the range inter-qubit coupling in easy-axis antiferromagnet-based 1D quantum registers through the correlation length variation near the quantum phase transition and/or near the antiferromagnetic resonance conditions. Our model of 1D nuclear quantum register corresponds to ferromagnetic transverse XX spin chain, but with not only pair interaction. It was shown that the nuclear two-spin correlation length may be raised to a great number of lattices constant.

We believe that the two-qubit operations, coherence state transfer and quantum states entanglement of far-separated qubits in the quantum register can be performed through similar long-range indirect coupling. It is not unlikely that entanglement may appear also for quantum states of opposite ends of spin chain giving the channel for entanglement transport across the chain.

We can consider also an ensemble variant of quantum register, which is made possible by the use of many moved apart in parallel working 1D spin chains.

The tuning of resonance frequencies of involved in quantum operation qubits may be performed through the imposition of local electrical gates. We do not discuss here special features of two-qubit decoherence for the far-separated spins-qubits states. Certain of related problems were discussed earlier in our book.\(^5\)

Note, that the external control of spin-wave excitations and propagation can play the role of the local measurements on the assisting electron spins, as this is required for localizable entanglement formation in 1D quantum registers with near neighbor interactions [6].

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