A switchable controlled-NOT gate in a spin-chain NMR quantum computer

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(Dated: March 31, 2022)

A method of switching a controlled-NOT gate in a solid-state NMR quantum computer is presented. Qubits of $I = 1/2$ nuclear spins are placed periodically along a quantum spin chain (1-D antiferromagnet) having a singlet ground state with a finite spin gap to the lowest excited state caused by some quantum effect. Irradiation of a microwave tuned to the spin gap energy excites a packet of triplet magnons at a specific part of the chain where control and target qubits are involved. The packet switches on the Suhl-Nakamura interaction between the qubits, which serves as a controlled NOT gate. The qubit initialization is achieved by a qubit initializer consisting of semiconducting sheets attached to the spin chain, where spin polarizations created by the optical pumping method in the semiconductors are transferred to the spin chain. The scheme allows us to separate the initialization process from the computation, so that one can optimize the computation part without being restricted by the initialization scheme, which provides us with a wide selection of materials for a quantum computer.

PACS numbers: 76.60.-k, 03.67.Lx, 75.45.+j

I. INTRODUCTION

A quantum computer (QC) is a Turing machine which performs information processing based on the principles of quantum mechanics. It makes the best use of the features of the quantum mechanics, such as superposition and entanglement of quantum states. These features enable us to perform parallel computation for all the possible states simultaneously, which makes it possible to deal with the problems that are formidable for classical (conventional) computers. New algorithms recently discovered have shown the great promise of the QC’s, which has accelerated the attempts to implement the QC’s in actual physical systems.

A QC is composed of a set of two-level systems called qubits. The qubits need to be isolated enough from the environment, and controllable from outside to deal with the information. In this respect, nuclear spin systems in a matter are the promising candidates, because they are only weekly coupled with the environment (electron systems) through hyperfine couplings, and controllable by the well-established technique of the nuclear magnetic resonance (NMR). Actually, the first 2-qubit QC’s were implemented by solution NMR. Kane proposed a multi-qubit NMR QC model, which utilizes $^{31}$P nuclei embedded in a Si matrix. This model provides us with a chance to extend the number of qubits systematically, whereas it requires fine structures to be fabricated and controlled, realization of which is a challenge to the current state-of-the-art nano-technology. On the other hand, Yamaguchi and Yamamoto proposed to utilize nuclei as they are in nature, i.e., in crystals. The $^{31}$P nuclei in CeP are placed in the magnetic field gradient, so that each nucleus (qubit) can be accessed by adjusting the NMR frequency. The proposal is very attractive because of its simple structure, although it still has some technical obstacles to be cleared. We have pursued this possibility checking the key issues.

One of the key issues is how to provide an inter-qubit (inter-nuclear) coupling, which is used for a controlled NOT (c-NOT) gate shown in Fig. 1. So far, a nuclear dipole (direct) coupling has been supposed to be a potential inter-qubit coupling. It is unfortunate, however, that the dipolar coupling is always present whenever qubits are put close to each other, so that one should continue applying the decoupling sequences to remove unwanted couplings. Apparently, these sequences consume a great deal of time, causing a longer computation time. Moreover, as the number of qubits is increased, the number of inter-nuclear couplings is increased accordingly, so that the decouplings become more and more complicated, and they eventually become formidable. So, a decoupling-free QC is highly desired, i.e., the inter-nuclear coupling should be able to be switched on when, and only when necessary.

Another key issue is the method of distinguishing, in the frequency domain, each nucleus (qubit) separated by a distance of the order of a lattice constant. Even the field gradient of $1 T/\mu m$ is still marginal for this purpose. The larger inter-nuclear (qubit) distance in the real space makes the distance between the adjacent NMR lines wider in the frequency domain, which relieves this

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constraint. Hence, the inter-nuclear coupling should be able to reach rather long distance. Unfortunately, the direct nuclear dipole coupling reaches at most a few lattice points [1].

These facts motivate us to seek for the possibility of the long range indirect couplings mediated by electrons. The indirect couplings include the J-coupling due to the covalent bondings, the RKKY interaction in metals [12], and the Suhl-Nakamura (SN) interaction in magnets [13, 14]. Among them, the SN interaction has the characteristics preferable for the present purpose, such as the long-range nature of the coupling and the external controllability of the coupling strength.

In this paper, we present details of the model of a solid-state NMR-QC with an inter-qubit coupling provided by the SN interaction [15]. A singlet-triplet transition in a quantum spin chain (1D antiferromagnet) provides us with a switch for the inter-qubit coupling. The model has the following advantages over the other existing models. (1) It is intuitive because the computation starts in the silent environments rather than the turbulence of interactions, which makes the designs of the logic gates simpler. (2) The long-range nature of the SN interaction allows us to place qubits apart farther from one another, which facilitates distinguishment of the qubits in the frequency domain. (3) The presence of the spin gap in the quantum spin chains allows simple operation of the gate switching compared to that proposed for the Kane’s type NMR-QC [15]. We also present the scheme of qubit initializer, an effective nuclear polarizer comprising the optical pumping and the polarization transfer methods. The scheme enables us to separate the materials responsible for the initialization and computation, so that one can optimize the computation part without being restricted by the initialization scheme.

**FIG. 1: Schematic view of the sequence for the c-NOT gate in the rotating frame of the target qubit. Upper and lower figures correspond to the cases of the up (0) and the down (1) states of the control qubit. (a) The target qubit spin is pointing to the Z-direction. The spin is rotated by a $\pi/2$ pulse around the negative X axis. (b) The spin starts to turn in the XY plane due to the additional field caused by the control qubit. (c) The spin turns by $\pm 90^\circ$ to positive or negative X direction in the XY plane. (d) The spin is rotated again by a $\pi/2$ pulse around the positive Y axis. The direction of the spin with respect to Z is hereby controlled according to the spin state of the control qubit.**

**FIG. 2: Schematic illustration of the c-NOT-gate switching in a 1D antiferromagnet in a magnetic field gradient. The $I = 0$ and $1/2$ (= qubits) nuclei are shown by balls and arrows, respectively. (1) All the inter-nuclear couplings are switched off in the absence of magnons. A $\pi/2$ pulse is applied to the target ($I_{N+1}$) qubit. (2) A magnon packet (hatched part) is excited between the control ($I_N$) and the target ($I_{N+1}$) qubits. The magnon packet entangles the two qubits, and the second $\pi/2$ pulse makes the $I_{N+1}$ spin turn either back to the +1/2 state for $I_N = 1/2$ (2a), or forth to the -1/2 state for $I_N = -1/2$ (2b) (see Fig. 1). The (2a) and (2b) states are superposed in the actual computation.**

**II. MODEL**

Here, we present the outline of the model. The main idea is illustrated in Fig. 1. The system consists of a one-dimensional array of electron spins (quantum spin chain) placed in a magnetic field gradient, which is produced by a micromagnet fabricated outside the spin chain [10]. Suppose that the electron spins are paired into singlets in the spin-Peierls systems. Also suppose that nuclei ($I = 1/2$) serving as qubits can be placed periodically, e.g., every ten lattice points, each of which has a hyperfine coupling with the electron spins.

Since there are no unpaired electron spins in the ground state, the nuclear spins are well-isolated from the environment. The nuclei are also decoupled from the charge and lattice properties of the electrons because $I = 1/2$. The rather long distance between qubit nuclei is effective both to diminish the direct nuclear dipole couplings between qubits and to distinguish one qubit from another in the NMR frequency domain, because the longer inter-qubit distance leads to larger interval between NMR lines in the given field gradient.

It is known that virtual exchanges of magnons between
nuclear spins result in the inter-qubit interaction called the Suhl-Nakamura (SN) interaction \[13, 14\]. Since it is not necessarily accompanied by actual excitations of magnons, it can exist even at temperatures well beneath the excitation gap. Nevertheless, the transverse component of the SN interaction with a form of \(I^y_j I^y_k\) is always absent in the field gradient because of the detuning effect, i.e., a mismatch in the Zeeman energies prevents the nuclei from exchanging magnons. On the other hand, the longitudinal component \((I^z_j I^z_k)\) of the SN interaction can survive even at low temperatures, which is characterized by the antiferromagnetic spin-spin correlation function in the ground state (see §IV) \[17, 18, 19\]. This interaction, however, is short-ranged because the spin-spin correlation function decays exponentially as a function of the distance, so that the interaction can reach only a few lattice points \[20\]. As a result, the interactions between nuclei apart from each other by the order of ten lattice points are completely switched-off at low temperatures.

In order for the system to work as a QC, one has to provide logic gates. A QC is complete if it is equipped with arbitrary rotation (R) and controlled-NOT (c-NOT) gates. \[21\] The R gate is a single qubit operation, which can be accomplished by an NMR pulse with an appropriate pulse width at the corresponding frequency. On the other hand, the c-NOT gate is a two-qubit operation, which works in such a way that a target qubit changes its logic according to the state of the control qubit, which can be realized by the pulse sequence shown in Fig. 1. Since the c-NOT gate between any combination of qubits apart from each other along the chain can be realized by a series of c-NOT gates between adjacent qubits \[22\], the QC is complete with the inter-nuclear coupling with the form \(I^z_j I^z_k\) between adjacent nuclear spins. This coupling is provided by the longitudinal component of the SN interaction via the \(k = 0\) magnon mode composed of the spin triplet state \[23\], which is selectively excited at a specific part of the chain where the c-NOT gate is to be performed.

The transition between singlet and triplet states by a microwave irradiation can be used to create the triplet \(k = 0\) magnons. Although the excitation is primarily forbidden for the usual electric dipolar transition, it often becomes possible in the actual systems because of some higher order terms in the electron-photon interaction Hamiltonians \[21, 22\]. The position of the excited magnons along the chain can be specified by the applied microwave frequency, which is uniquely given in the field gradient. The energy diagrams of the \(k = 0\) magnon excitations in the magnetic field is shown in Fig. 3 \[23, 24\]. In the field gradient, the magnetic field at each part of the chain is unique so that the excitation energy to the lowest triplet state \((|1\rangle\rangle - 1\rangle\rangle)\) is also uniquely given, which provides us with a spatial resolution of the excitation, i.e., one can specify the position of the magnon excitations by adjusting the frequency of the applied microwave. The region and the amplitude of the excited magnons can be controlled by the frequency resolution and the power of the microwave.

Since the two upper states \((|10\rangle\rangle, |11\rangle\rangle)\) irrelevant to the transition of interest can be ignored, one can introduce effective spins within the \(|00\rangle\rangle\) and \(|01\rangle\rangle\) subspace \[26\]. These spins are rotated by the microwave, creating a packet of superpositions of \(|00\rangle\rangle\) and \(|1\rangle\rangle - 1\rangle\rangle\) along the chain \[24\], corresponding to the magnon excitations with the wave number \(k \sim 0\). The packet is localized along the chain due to the magnetic field gradient (see §III). The number of excited spins is given by the balance between the excitation to the \(|1\rangle\rangle - 1\rangle\rangle\) state and the relaxation (with the lifetime of \(T_2\)) to the ground state.

The triplet states make an additional field \(\left(H_{tr}\right)\) associated with the “shift” at the qubit site, which should be distinguished from the additional field from the adjacent qubit via the SN interaction \(\left(H_{SN}\right)\). Assuming the hyperfine coupling \(A_0 = 100 \text{ kOe/} \mu_B\) and the rotation of the spins: \(n(0) \sim 1\%\), \(H_{tr}\) is estimated to be \(\sim 1 \text{ kOe}\), which corresponds to a \(1\%\) shift of the NMR frequency in the magnetic field of 10 T. In practice, the exact value of \(H_{tr}\) can be measured by the following method; under the microwave irradiation, one observes the shift of the NMR frequency of the target qubit while saturating the control qubit by applying the corresponding NMR rf field continuously. The saturation of the control qubit results in \(H_{SN} = 0\) at the target qubit, so that the observed shift directly corresponds to \(H_{tr}\).

Then, the c-NOT gate is achieved as follows (see Fig. 1): (a) In the beginning, the target qubit \((I_{N+1})\) is assumed to be pointing to the Z direction. The \(\pi/2\) pulse with the rf frequency \(\omega = \gamma_n H(x_{N+1})\) is applied in the negative X direction in the rotating frame of the target qubit. (b) A microwave is applied to the chain. The SN interaction is switched on, and the target qubit starts to rotate in the XY plane of the rotating frame with \(\omega = \gamma_n (H(x_{N+1}) + H_{tr})\). The direction of the rotation...
with respect to the frame depends on the state of the control qubit \( I_{N} \). (c) By the time \( t = \pi/(2\gamma_{n}H_{SN}) \), the target qubit reaches either positive or negative X. (d) The SN interaction is shut off by shutting off the microwave, and the second \( \pi/2 \) pulse with \( \gamma_{n}H(x_{N+1}) \) is applied in the negative Y direction, which rotates the target qubit upward or downward according to the control qubit. This sequence allows us to perform the c-NOT gate.

III. SINGLET-TRIPLET EXCITATIONS IN THE QUANTUM SPIN CHAIN

One of the key phenomena in the present model is the selective excitations of the triplet states shown in Fig. 3. Let us see the excitation in detail. We consider the selective excitations of the triplet states shown in Fig. 3 as an example, and follow the description in Ref. 24. The effective spin is introduced within the subspace consisting of the ground state \( |00\rangle \) and the lowest excited state \( |1\rangle \). This treatment is helpful to visualize the transition as a rotation of the spins. The Hamiltonians which govern the system are,

\[
H = H_{0} + H_{1},
\]

\[
H_{0} = J \sum_{i} S_{i1} \cdot S_{i2} + g \mu_{B} \sum_{i} H(x_{i}) \cdot (S_{i1} + S_{i2}),
\]

\[
H_{1} = J_{1} \sum_{nn} S_{i1} \cdot S_{j1} + J_{1} \sum_{nn} S_{i2} \cdot S_{j2},
\]

Here, \( J \) and \( J_{1} \) are the intra- (rung) and inter-pair (leg) exchange interactions, respectively. \( H(x_{i}) \) is the external field at the \( i \)-th site and “nn” means the nearest neighbor sites. By introducing the operators \( S_{i} = s_{i1} = s_{i2} \) and \( T_{i} = s_{i1} - s_{i2} \), Eqs. (1)~(3) are rewritten as,

\[
H_{0} = \frac{1}{2} J \sum_{i} S_{i}^{2} + g \mu_{B} \sum_{i} H(x_{i}) \cdot S_{i},
\]

\[
H_{1} = \frac{1}{2} J_{1} \sum_{nn} (S_{i} \cdot S_{j} + T_{i} \cdot T_{j}),
\]

where some constant terms are dropped.

We further rewrite these Hamiltonians in terms of the Pauli spin components in the following manner.

\[
S_{i}^{x} = 1 - \sigma_{i}^{z}, \quad S_{i}^{y} = S_{i}^{z} = 0, \quad S_{i}^{z} = \frac{1}{2}(\sigma_{i}^{z} - 1),
\]

\[
T_{i}^{x} = \frac{1}{\sqrt{2}} \sigma_{i}^{y}, \quad T_{i}^{y} = \frac{1}{\sqrt{2}} \sigma_{i}^{x}, \quad T_{i}^{z} = 0.
\]

As a consequence of these transformations, the two states of \( |00\rangle \) and \( |1\rangle \) can be treated as the two spin states represented by the Pauli spin matrices. The total Hamiltonian, Eq. (1) is expressed by these spin matrices as,

\[
H = \frac{N}{2} (J + J_{1}/4 - g \mu_{B} \sum_{i} H(x_{i}))
\]

\[
- \frac{1}{2} \sum_{i} \{ J + J_{1}/4 - g \mu_{B} H(x_{i}) \} \sigma_{i}^{z}
\]

\[
+ \frac{J_{1}}{8} \sum_{nn} \{ 2(\sigma_{i}^{x} \sigma_{j}^{x} + \sigma_{i}^{y} \sigma_{j}^{y}) + \sigma_{i}^{z} \sigma_{j}^{z} \}
\]

This describes the system of the spins coupled through anisotropic exchange interactions. The microwave rotates these spins.

The small-angle rotations of the spins in a small region create a packet of \( k \sim 0 \) magnons like a soliton. The packet is localized on the chain due to the magnetic field gradient. A mismatch in the magnon excitation energies between adjacent regions along the chain prohibits the packet from moving to the lower field region. On the other hand, the continuum excitations near the one-magnon excitations at \( k=0 \) is absent, so that it is difficult for the packet to move to the higher field region unless the process of the energy release by phonon emissions is considerable. Consequently, the magnons are confined in the region where they are excited, and the SN interaction is produced only between the qubit pair of interest.

The population of the magnons with \( k = 0 \) \((\equiv n(0))\) is determined by the balance between excitation and relaxation,

\[
\frac{dn(0)}{dt} = W_{ex} - \frac{n(0)}{T_{x}},
\]

where \( W_{ex} \) is the transition probability of \( |00\rangle \rightarrow |1\rangle \) per unit time by the microwave irradiation, and \( T_{x} \) is the magnon lifetime. At the steady state, \( dn(0)/dt = 0 \), so that \( n(0) = W_{ex} T_{x} \). As the microwave irradiation is shut off, the spins start to relax to the ground state \( \sigma_{z} = -1 \) with the relaxation time given by \( T_{x} \).

We end up this section with some remarks on the nature of the excited states. One is about the lifetime of the excited states \( T_{x} \); it could be rather long because the excitation is primarily forbidden for the usual electric dipolar transition. Although the forbiddance itself is usually lifted by some additional interactions such as the Dzyaloshinsky-Moriya interaction, the primarily forbidden transition is expected to lead to rather long lifetime of the excited triplet states and narrower transition line, which is favorable for the selective excitation. Another is about the wave number of the triplet states; they should have \( k=0 \) and the transition to the staggered component \( (k = a/\pi) \) is forbidden, because only the transitions with the momentum transfer \( q \equiv k - k' = 0 \) are allowed by the microwave, and the ground state \((|00\rangle)\) is
a uniform singlet state \((k=0)\). This fact is quite favorable for the long-range inter-nuclear coupling with \(q \sim 0\). Note that the magnons excited by the microwave are in the non-equilibrium states far from the thermal equilibrium where the \(k = a/\pi\) magnons are primarily excited.

### IV. INTER-NUCLEAR COUPLINGS MEDIATED BY MAGNONS

We next look into the details of the longitudinal component of the SN interaction caused by a packet of spin triplet states. For simplicity, we assume the following on-site anisotropic hyperfine Hamiltonian in the \(i\)-th site,

\[
H_{hf} = \{A_i s_{1i}^z I_i^z + \frac{1}{2} A_\perp (s_{1i}^+ I_i^- + s_{1i}^- I_i^+)\}
\]  

(9)

which can be rewritten using the spin introduced in Eq. (3) as,

\[
H_{hf} = \frac{1}{4} A_i I_i^z \sigma_i^z - \frac{1}{2} A_\perp (\sigma_i^+ I_i^- + \sigma_i^- I_i^+)\]

(10)

Hence, besides the term, \(-\frac{1}{2} A_i I_i^z\), which can be incorporated into the Zeeman term in the nuclear Hamiltonian, the nuclear interaction with the spin \(\sigma\) can be expressed by the anisotropic hyperfine interaction. The first term creates the shifts at the nuclear sites corresponding to \(H_{hf}\) and the SN interactions, and the other terms give rise to the spin-lattice relaxation [32, 33, 34]. The effect of the spin lattice relaxation is discussed in the next section.

Since the transverse component of the SN interaction due to \(\sigma^\pm\) vanishes in the field gradient, we can restrict ourselves to the longitudinal component. The longitudinal component of the SN interaction is given by,

\[
H_{SN} = W_{ij} I_i^z I_j^z,
\]

(11)

where,

\[
W_{ij} = \left(\frac{\gamma_n A_i}{N}\right)^2 \sum_{k,k',k\neq k'} \frac{n_k - n_{k'}}{\epsilon_k - \epsilon_{k'}} \cos\{(k - k')r_{ij}\}.
\]

(12)

Here, \(n_k\) and \(\epsilon_k\) are, respectively, the population and the energy of the magnon with the wave number \(k\), and \(r_{ij}\) is the distance between the two nuclei of interest. In the equilibrium states, \(n_k\) is given by the Bose function for the given temperature.

Actually, eq. (11) is a special case of the general formulas for the indirect spin-spin interaction,

\[
H_{ind} = \Phi(r_{ij}) I_i^z I_j^z,
\]

(13)

with the range function,

\[
\Phi(r_{ij}) = \frac{\gamma_n^2 A_i^2}{\pi} \sum_q \chi(q) \exp(iqr_{ij}).
\]

(14)

Here, \(\chi(q)\) is the zero energy component of the generalized susceptibility, and \(q = k - k'\). In the present case, the electronic state is not in the equilibrium state, so that \(\chi(q)\) is different from that in the thermal equilibrium. Note in particular, that the magnons with the wave numbers other than \(k \sim 0\), such as \(k = \pi/a\), are not excited here.

The range to which this interaction reaches depends on the range function, which is determined by the form of \(\chi(q)\) as a function of \(q\). For the pair of nuclei far from each other, the most important interaction comes from the uniform part of the susceptibility, i.e. \(q \sim 0\) caused by the scatterings of the magnons with \(k \sim 0\).

In the case of the transverse component of the SN interaction in a 3-D system, the range function can be calculated only from the magnon dispersions and has the form \(\sim a/r \exp(-r/3a)\) (\(a\) is a lattice constant) [3]. In our case, however, the situation is completely different from this case, and the interaction reaches rather long distance because of the following reasons. Firstly, in the longitudinal component, the number of excited magnons, as well as the magnon dispersions, are responsible for the range function (see Eq. (12)). Secondly, the system is 1-D so that a qualitative difference exists in the structures of \(\chi(q)\). Thirdly, the system is not in the equilibrium state. Since \(\chi(q)\) is enhanced at \(q \sim 0\) in the present case, a rather long distance interaction is expected between the nuclei of interest. Note again that the contribution from the magnons with \(k \sim \pi/a\) to \(\chi(q \sim 0)\), which exists in the equilibrium state, does not exist in the present case.

Here, we make a rough estimation of the range function for the case of Fig. 4 using Eq. (12). The magnon dispersion of the triplet state in this situation is given by [35],

\[
\epsilon(k_n) = C + J(j_1 - \frac{1}{4} j_3^3) \cos(k_n) + ...
\]

(15)

where \(k_n = n\pi/N\), \(j_1 = J_1/J\) and \(C\) is the part independent of \(k_n\). Here, the magnetic field is assumed to be uniform in this region. Using Eq. (15) and recalling that the microwave irradiation excites only the \(k = 0\) component of the magnons, i.e., \(n(k) = 0\) for \(k \neq 0\), one can calculate the range function \(W_{ij}\) in Eq. (12),

\[
W_{ij} = \left(\frac{\gamma_n A_i}{N}\right)^2 \sum_{n=1}^N \frac{2n(0)}{\epsilon(k_n) - \epsilon(0)} \cos(k_n r_{ij})
\]

\[
= \frac{2\gamma_n^2 A_i^2 (n(0)/N)}{J(j_1 - \frac{1}{4} j_3^3)N} \sum_{n=1}^N \cos(k_n r_{ij})\]

(16)

Assuming \(N = 20\), \(r_{ij} = 10\) (in units of \(a\)), \(A_i = 100\) kOe/\(\mu\)B, \(\gamma_n/(2\pi) = 4.3\) MHz/kOe (\(^1\)H as an example), \(J = 50\) K, \(j_2 = 0.2\) and \(n(0)/N = 0.01\), one obtains \(W_{ij} = 15\) kHz, which is the same order of magnitude as the nuclear dipole coupling acting between nuclei 3 A apart from each other [3, 4], and one to three orders of magnitude greater than the J-couplings used in the solution NMR-QC’s [5, 6].
The estimation here is for the ideal case, because the population difference may be underestimated \((n(k \neq 0))\) may be populated somewhat in the actual situation. Moreover, the realistic magnon dispersions as well as the conditions of the microwave excitation such as \(n(0)/N\) and \(N\) may affect the value of \(W_{ij}\). Nevertheless, this estimation indicates that the longitudinal component of the SN interaction could be large enough to serve as a c-NOT gate. Note that the strength of the coupling, \(W_{ij}\), can be controlled by the microwave intensity via \(n(0)\), because it is determined by the balance between excitation and relaxation, and in the steady state, \(n(0) = W_{ex}T_s\).

V. DECOHERENCE

Decoherence is one of the serious concerns in this model. On the one hand, the excited triplet states can create inter-qubit couplings, but on the other hand, they inevitably activate the scattering channels of the nuclear spins and reduce the spin-lattice relaxation time \(T_1\) [32, 33]. Although this is unavoidable, it is still possible to reduce the chances of decoherence.

Let us see the scattering process of magnons by a nucleus in detail. Since the direct one-magnon process is prohibited because of the mismatch between nuclear and electron excitation energies, the possible lowest order process is the two-magnon (Raman) process. This process can be the major cause of \(T_1\) relaxation when the number of excited magnons is increased. The process is known, however, to require highly anisotropic exchange interactions because of the conservation of the angular momentum before and after the scattering. Hence, the process can be reduced in the system with isotropic exchange interactions [32, 33]. The three-magnon process is the next possible process, where two incident magnons are scattered by a nucleus and one magnon is emitted. This process is active even in the case of isotropic exchange interactions.

In general, the spin-lattice relaxation time is given by,

\[
\frac{1}{T_1} = \frac{2\omega_n^2 A_1^2 k_B T}{g^2 \mu_B^2} \sum_q \frac{\text{Im} \chi^+(q, \omega_n)}{\omega_n}.
\]  

(17)

Here, \(\chi^+(q, \omega)\) is the transverse component of the dynamical susceptibility and \(\omega_n\) is the NMR frequency. (Note again, that the present situation is not a thermal equilibrium state, so that \(\chi(q, \omega)\) is different from those in the thermal equilibrium.) As seen in Eq. (17), \(1/T_1\) is proportional to \(A_1^2\). Recalling that \(A_\parallel\) is the only necessary component of the hyperfine coupling for the longitudinal component of the SN interaction, the highly anisotropic hyperfine coupling \((A_\parallel/A_\perp \gg 1)\) may be used to reduce \(1/T_1\) without reducing the longitudinal component of the SN interaction. Such highly anisotropic hyperfine interaction can be realized by transferred hyperfine couplings [34].

Even with such effects, however, it might be inevitable to invoke the quantum error correction method for the unavoidable nuclear spin flips in the end [37, 38]. Even so, the chain structure is fortunate for the error correction process. The error correction requires three equivalent QC’s, which are entangled like \(\alpha_1\alpha_2\alpha_3\) at each qubit \(l\), where \(\alpha_i\) is an eigensate (e.g. spin-up state) at the qubit \(l\) of the \(i\)-th QC. Such set of nuclei can be provided by the three consecutive chains. It is possible to align the qubit nuclei (see [37] and once they are aligned, the inter-chain nuclear dipole couplings keep them entangled. (For this purpose, only the \(I^+I^-\) component is needed. Since \(I^+I^-\) components make the NMR line broad, they should be eliminated by applying a small field gradient in this direction.)

VI. NUCLEAR ALIGNMENTS

So far, we have described the model for a single QC. Unfortunately, the sensitivity of the conventional NMR method is not high enough to detect signals from a single QC, so that one needs to integrate many equivalent QC’s to obtain the results of computations. In this process, the nuclear alignment can help us to reduce the number of equivalent nuclei required for each qubit. It is also advantageous for obtaining a narrower NMR line.

The nuclear alignment is also associated with the qubit initialization. Although the qubit initialization may be achieved by the pseudo-pure state technique [33] and/or the algorithmic cooling [40, 41], aligning nuclear spins, even partially, can assist the methods to work in the systems with the large number of qubits \((N)\), because the number of QC’s which happen to be in the pure state in the thermal equilibrium is proportional to \((\hbar \omega_n/2k_B T)N/2^N\), which becomes smaller and smaller as increasing \(N\). The nuclear alignment can relieve this problem.

Here, we propose a possible configuration of a “qubit initializer”, which partially aligns the qubits in the spin chains by the optical pumping technique [42]. The scheme enables us to separate the materials responsible for the initialization and computation, so that one can optimize the computation part without being restricted by the initialization scheme. The schematic illustration is shown in Fig. 3. Films made of spin chains are sandwiched by Si single crystals and placed in a field gradient and at a low temperature. The electrons in the semiconducting Si matrix are polarized by a circularly polarized near-infrared laser light with an energy corresponding to the semiconducting gap of Si [43, 44], and the polarizations of the electrons are transferred to the nuclear spin systems of the spin chains through the hyperfine couplings [45, 46, 47] or the cross-polarization /coherent transfer techniques [45]. Here, the films and the Si matrix are not necessarily bonded chemically but contacted mechanically, because the direct dipolar couplings are available for the polarization transfer process [42].

After the nuclear alignment is completed, the laser
light is shut off. The excited electrons in the Si matrix will die out quickly and the Si matrix will return to the silent environment. Here, the Si matrix is selected because the abundant nuclei (I = 0). Since the optical pumping is effective in most of the semiconductors [4], other semiconductors with no nuclear spins can be used as well. For example, CdTe enriched by the isotopes with no nuclear spins, such as 110,112,114Cd and 126,128,130Te is also available.

VII. PRACTICAL ISSUES IN THE IMPLEMENTATION

We have shown an ideal model for the NMR QC so far, but one might notice some practical issues to implement this model. First of all, one should find a suitable spin chain system with a singlet ground state, containing more than two stable isotopes for one element, one of which has I = 1/2. Moreover, the periodical placements of the 1/2 nuclear spins may require some ingenious techniques.

One of the possible candidates for the QC would be a film made of some organic materials with spin gaps. They contain 1H and 13C having I = 1/2. They also have large unit cells, which are useful to reserve large spacial distances between qubits. Moreover, one could utilize a well-established chemical technique of the selective isotope replacement of 1H by 2D (I = 1) [14] or 12C (I = 0) by 13C (I = 1/2). The periodical placements of the qubits may be achieved with the epitaxial growth [15] and/or the Langmuir-Blodgett methods as follows. One prepares two sets of molecules with the same chemical formulas but different isotopes by the selective isotope replacement technique, for example, all deuterized samples and those having 1H's at one of the hydrogen sites. These two sets of molecules could be layered epitaxially using the MBE or the Langmuir-Blodgett method so as for 1H's or 13C's to be placed periodically.

In order to avoid unnecessary nuclear couplings, the nuclei other than qubits are preferable to have no spins (I = 0). In this sense, it is fortunate that major abundant isotopes in organic materials such as 12C and 16O have no spins. The Haldane systems such as NENP and NINO are also fortunate because they contain 58Ni, an abundant isotope with no spins. In addition, a high power decoupler and/or a decoupling sequence between unlike spins using a train of π-pulses can counteract the effects of the nuclei with I ≠ 0 such as 2D.

Acknowledgments

We wish to acknowledge helpful advices by G. Kido and M. Kitagawa. This work has been supported by CREST of JST (Japan Science and Technology Corporation).

[1] D. Deutsch, Proc. R. Soc. Lond. A 400, 97 (1985).
[2] P. W. Shor, SIAM, J. Compt. 26, 1417 (1997).
[3] L. K. Grover, Phys. Rev. Lett. 80, 4329 (1998).
[4] I. L. Chuang, N. Gershenfeld, and M. Kubinec, Phys. Rev. Lett. 80, 3408 (1998).
[5] J. A. Jones and M. Mosca, J. Chem. Phys. 109, 1648 (1998).
[6] B. E. Kane, Nature 393, 133 (1998).
[7] F. Yamaguchi and Y. Yamamoto, Appl. Phys. A 68, 1 (1999).
[8] K. Hashi, T. Shimizu, A. Goto, H. Kitazawa, G. Kido, and T. Suzuki, Appl. Phys. A 70, 359 (2000).
[9] T. D. Ladd, J. R. Goldman, F. Yamaguchi, and Y. Yamamoto, Appl. Phys. A 71, 27 (2000).
[10] J. R. Goldman, T. D. Ladd, F. Yamaguchi, and Y. Yamamoto, Appl. Phys. A 71, 11 (2000).
[11] A. Goto, T. Shimizu, R. Miyabe, K. Hashi, H. Kitazawa, G. Kido, K. Shimamura, and T. Fukuda, Appl. Phys. A 74, 73 (2002).
[12] M. A. Ruderman and C. Kittel, Phys. Rev. 96, 99 (1954).
[13] H. Suhl, Phys. Rev. 109, 606 (1958).
[14] T. Nakamura, Prog. Theor. Phys. 20, 542 (1958).
[15] A. Goto, T. Shimizu, and K. Hashi (2002), quant-ph/0201060.
[16] A. Khitun, R. Ostroumov, and K. L. Wang, Phys. Rev. A 64, 62304 (2001).
[17] M. Itoh, M. Sugahara, T. Yamauchi, and Y. Ueda, Phys. Rev. B 54, R9631 (1996).
[18] A. W. Sandvik, E. Dagotto, and D. J. Scalapino, Phys. Rev. B. 53, R2934 (1996).
[19] J. Kishine, J. Phys. Soc. Jpn. 66, 1229 (1997).
[20] S. R. White, R. M. Noack, and D. J. Scalapino, Phys. Rev. Lett. 73, 886 (1994).
[21] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, and H. Weinfurter, Phys. Rev. A 52, 3457 (1995).
[22] D. Collins, K. W. Kim, W. C. Holton, H. Sierzputowska-Gracz, and E. O. Stejskal, Phys. Rev. A 62, 22304 (2000).
[23] V. Zevin and N. Kaplan, Phys. Rev. B 12, 4604 (1975).
[24] T. M. Brill, J. P. Boucher, J. Voiron, G. Dhalenne, A. Revcolevschi, and J. P. Renard, Phys. Rev. Lett. 73, 1545 (1994).
[25] W. Lu, J. Tuchendler, M. von Ortenberg, and J. P. Renard, Phys. Rev. Lett. 67, 3716 (1991).
[26] M. Tachiki and T. Yamada, J. Phys. Soc. Jpn. 28, 1413 (1970).
[27] D. Augier and D. Poilblanc, Eur. Phys. J. B 1, 19 (1998).
[28] G. S. Uhrig and H. J. Schulz, Phys. Rev. B 54, R9624 (1996).
[29] A. W. Garrett, S. E. Nagler, D. A. Tennant, B. C. Sales, and T. Barnes, Phys. Rev. Lett. 79, 745 (1997).
[30] W. Yu and S. Haas, Phys. Rev. B 62, 344 (2000).
[31] B. Grenier, L. P. Regnault, J. E. Lorenzo, J. P. Boucher, A. Hiess, G. Dhalenne, and A. Revcolevschi, Phys. Rev. B 62, 12206 (2000).
[32] D. Beeman and P. Pincus, Phys. Rev. 166, 359 (1968).
[33] M. W. Pieper, J. Kotzler, and K. Nehrke, Phys. Rev. B 47, 11962 (1993).
[34] D. A. Ivanov and P. A. Lee, Phys. Rev. B 59, 4803 (1999).
[35] M. Muller and H.-J. Mikeska, J. Phys. Condens. Matter 12, 7633 (2000).
[36] F. Mila and T. M. Rice, Physica C 157, 561 (1989).
[37] P. Shor, Phys. Rev. A 52, 2493 (1995).
[38] A. M. Steane, Phys. Rev. Lett. 77, 793 (1996).
[39] N. A. Gershenfeld and I. L. Chuang, Science 275, 350 (1997).
[40] T. D. Ladd, J. R. Goldman, F. Yamaguchi, Y. Yamamoto, E. Abe, and K. M. Itoh (2001), quant-ph/0109039.
[41] L. J. Schulman and U. V. Vazirani, Proc. 31st ACM Symp. on Theory of Computing p. 322 (1999).
[42] R. Tycko, Sol. State Nucl. Mag. Res. 11, 1 (1998).
[43] G. Lampel, Phys. Rev. Lett. 20, 491 (1968).
[44] F. Meier and B. P. Zakharchenya, eds., Optical Orientation, vol. 8 of Modern Problems in Condensed Matter Science (North Holland, Amsterdam, 1984).
[45] C. A. Michal and R. Tycko, Phys. Rev. Lett. 81, 3988 (1998).
[46] C. A. Michal and R. Tycko, Phys. Rev. B 60, 8672 (1999).
[47] W. Farah, M. Dyakonov, D. Scalbert, and W. Knap, Phys. Rev. B 57, 4713 (1998).
[48] C. P. Slichter, Principles of Magnetic Resonance, vol. 1 of Springer Series of Solid State Sciences (Springer Verlag, Berlin, 1990).
[49] S. Aonuma, H. Sawa, Y. Okano, R. Kato, and H. Kobayashi, Synth. Metal. 58, 29 (1993).
[50] T. J. Schuerlein, A. Schmidt, P. A. Lee, K. W. Nebesny, and N. R. Armstrong, Jpn. J. Appl. Phys. 1 34, 3837 (1995).