Numerical simulation of a controlled–controlled-not (CCN) quantum gate in a chain of three interacting nuclear spins system

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Abstract

We present a study of a quantum controlled–controlled-not gate, implemented in a chain of three nuclear spins weakly Ising interacting between all of them, that is, taking into account first and second neighbour spin interactions. This implementation is done using a single resonant $\pi$-pulse on the initial state of the system (digital and superposition). The fidelity parameter is used to determine the behaviour of the CCN quantum gate as a function of the ratio of the second neighbour interaction coupling constant to the first neighbour interaction coupling constant ($J'/J$). We found that for $J'/J \geq 0.02$ we can have a well-defined CCN quantum gate.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

There is no doubt that the discovery of the polynomial time solution of the prime factorization problem (Shor’s algorithm [1]) and the fastest data base searching (Grover’s algorithm [2]) by a quantum computer, and the importance of the implementations of these algorithms in cryptography analysis [3], have made the study of the physical realization of a quantum computer a priority for many researchers [4, 5]. A quantum computer works with qubits instead of bits, where a qubit is the superposition of two quantum levels of the system which are defined as $|0\rangle$ and $|1\rangle$, and a tensorial product of these states makes up a register. Although one could say that there are already quantum computers with registers of a few qubits [6], these are still far too low for serious studies (which may require at least 100-qubit registers, that is, at least a $2^{100}$ dimensional Hilbert space). In addition, much more technological development (or a very neat idea) is needed to have a really powerful quantum computer. One model of a solid state quantum computer which looks promising due to advances in single spin measurements [7] is that of a chain of nuclear spins quantum computer [4, 8], where the Ising interaction between first neighbours is considered. This interaction allows us to ideally...
implement this type of computer up to 1000 qubits or more [9]. First neighbour interaction between spins also allows us to implement a Controlled-Not (CN) quantum gate using a single \( \pi \)-pulse [10]. However, the implementation of a Controlled–Controlled-Not (CCN) quantum gate, which is needed in Shor’s factorization, Grover’s searching and full-adder algorithms [11], is not that simple. In addition, the CCN quantum gate is also important since it has a universality characteristic [12]. The CN and CCN gates are defined classically by the following two tables [13]:

| CN | \( a \) | \( b \) | \( a' \) | \( b' \) |
|----|-----|-----|-----|-----|
| 0  | 0   | 0   | 0   | 0   |
| 0  | 1   | 0   | 1   | 0   |
| 1  | 0   | 1   | 1   | 0   |
| 1  | 1   | 1   | 0   | 1   |

| CCN | \( a \) | \( b \) | \( c \) | \( a' \) | \( b' \) | \( c' \) |
|-----|-----|-----|-----|-----|-----|-----|
| 0  | 0   | 0   | 0   | 0   | 0   | 0   |
| 0  | 0   | 1   | 0   | 0   | 0   | 1   |
| 0  | 1   | 0   | 0   | 1   | 0   | 0   |
| 0  | 1   | 1   | 0   | 0   | 1   | 1   |
| 1  | 0   | 0   | 1   | 0   | 1   | 0   |
| 1  | 0   | 1   | 1   | 0   | 1   | 0   |
| 1  | 1   | 0   | 1   | 1   | 0   | 1   |
| 1  | 1   | 1   | 1   | 1   | 1   | 0   |

where \( a \) (called the control bit) and \( b \) (called the target bit) for CN (\( a, b \) and \( c \) for CCN) represent the input information, and \( a' \) and \( b' \) (\( a', b' \) and \( c' \) for CNN) represent the output information. In a CN gate, \( b' \) (target) changes if and only if \( a \) (control) has the value 1. In a CCN gate, \( c' \) changes if an only if \( a \) and \( b \) have the value 1. The ideal CN and CCN quantum gates, operating on an arbitrary L-register \(|i_{L−1},\ldots,i_a,\ldots,i_b,\ldots,i_c,\ldots,i_0\rangle\) (where \( i_j = 0, 1 \)), would be defined as

\[
\text{CN}_{ab}|i_{L−1},\ldots,i_a,\ldots,i_b,\ldots,i_c,\ldots,i_0\rangle = |i_{L−1},\ldots,i_a,\ldots,i_b \oplus i_a,\ldots,i_c,\ldots,i_0\rangle
\]

and

\[
\text{CCN}_{abc}|i_{L−1},\ldots,i_a,\ldots,i_b,\ldots,i_c,\ldots,i_0\rangle
\]

\[
= |i_{L−1},\ldots,i_a,\ldots,i_b,\ldots,i_c \oplus (i_a \cdot i_b),\ldots,i_0\rangle,
\]

where the operation \( \oplus \) means summation module 2. In this paper we consider second neighbour interaction between spins in the one-dimensional chain of spins quantum computer, and we show that it is possible to implement a CCN quantum gate with just a single \( \pi \)-pulse. Of course, a CN quantum gate continues to be represented by a single \( \pi \)-pulse.

2. Equation of motion

Consider a one-dimensional chain of three equally spaced nuclear-spins systems (spin 1/2) making an angle \( \cos \theta = 1/\sqrt{3} \) with respect to the \( z \)-component of the magnetic field (chosen...
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in this way to kill the dipole–dipole interaction between spins) and having an rf-magnetic field in the transversal plane. The magnetic field is given by

\[ \mathbf{B} = (b \cos \omega t, -b \sin \omega t, B(z)), \]  

(1)

where \( b \) is the amplitude of the rf-field, \( B(z) \) is the amplitude of the \( z \)-component of the magnetic field, \( \omega \) is the angular frequency of the rf-field (its phase has been chosen as zero for simplicity). So, the Hamiltonian of the system is given by

\[ H = -\sum_{k=0}^{2} \mu_k \cdot \mathbf{B}_k - 2J\hbar \sum_{k=0}^{1} I^z_k I^z_{k+1} - 2J'h \sum_{k=0}^{0} I^z_k I^z_{k+2}, \]  

(2)

where \( \mu_k \) represents the magnetic moment of the \( k \)-th nucleus which is given in terms of the nuclear spin as

\[ \mu_k = \hbar \gamma (I^x_k, I^y_k, I^z_k), \]  

\( \gamma \) being the proton gyromagnetic ratio.

\( \mathbf{B}_k \) represents the magnetic field at the location of the \( k \)-th spin. The second term in the right-hand side of (2) represents the first neighbour spin interaction, and the third term represents the second neighbour spin interaction. \( J \) and \( J' \) are the coupling constants for these interactions. This Hamiltonian can be written in the following way:

\[ H = H_0 + W, \]  

(3a)

where \( H_0 \) and \( W \) are given by

\[ H_0 = -\hbar \left\{ \sum_{k=0}^{1} \omega_k I^z_k + 2J \left( I^z_0 I^z_1 + I^z_1 I^z_2 \right) + 2J' \left( I^z_0 I^z_2 \right) \right\}, \]  

(3b)

and

\[ W = -\frac{\hbar \Omega}{2} \sum_{k=0}^{1} \left[ e^{i\omega t} I^+_k + e^{-i\omega t} I^-_k \right]. \]  

(3c)

Here, \( \omega_k = \gamma B(z_k) \) is the Larmor frequency of the \( k \)-th spin, \( \Omega = \gamma b \) is Rabi’s frequency, and \( I^\pm_k = I^x_k \pm iI^y_k \) represents the ascend operator (+) or the descend operator (−). The Hamiltonian \( H_0 \) is diagonal on the basis \( \{|i_2 i_1 i_0\rangle\} \) with \( i_j \neq 0, 1 \) (zero for the ground state and one for the exited state),

\[ H_0|i_2 i_1 i_0\rangle = E_{i_2 i_1 i_0} |i_2 i_1 i_0\rangle. \]  

(4a)

The eigenvalues \( E_{i_2 i_1 i_0} \) are given by

\[ E_{i_2 i_1 i_0} = \frac{-\hbar}{2} \left\{ (-1)^{i_2} \omega_0 + (-1)^{i_1} \omega_1 + (-1)^{i_0} \omega_0 + J[(-1)^{i_2} \omega_1 + (-1)^{i_1} \omega_0 + J'[(-1)^{i_2} \omega_1 + (-1)^{i_1} \omega_0 + J']. \right\} \]  

(4b)

The term (3c) of the Hamiltonian (3a) allows us to have single spin transitions on the above eigenstates by choosing the proper resonant frequency, as shown in figure 1. For example, if we are interested in having the transition \( |110\rangle \leftrightarrow |111\rangle \), since this represents the CCN quantum gate operation, according to table 2, the resonant frequency would be

\[ \omega = \omega_0 - J - J'. \]  

(5)

Of course, we could also have considered a CCN quantum gate as defined by the transition \( |011\rangle \leftrightarrow |111\rangle \), by defining the order of the elements differently.

To solve the Schrödinger equation

\[ i\hbar \frac{\partial \Psi}{\partial t} = H\Psi, \]  

(6)

let us propose a solution of the form

\[ \Psi(t) = \sum_{k=0}^{2} C_k(t)|k\rangle, \]  

(7)
where we have used decimal notation for the eigenstates in (4a), $H_0|k\rangle = E_k|k\rangle$. Substituting (6) in (5), multiplying for bra $\langle m|$, and using the orthogonality relation $\langle m|k\rangle = \delta_{mk}$, we get the following equation for the coefficients:

$$i\hbar \dot{C}_m = E_m C_m + \sum_{k=0}^{7} C_k \langle m|W|k\rangle m = 0, \ldots, 7.$$  

(8)

Now, using the following transformation

$$C_m = D_m e^{-iE_m t/\hbar},$$  

(9)

the fast oscillation term $E_m C_m$ of equation (8) is removed (this is equivalent to going to the rotating frame of reference), and the following equation is obtained for the coefficients $D_m$

$$i\dot{D}_m = \frac{1}{\hbar} \sum_{k=0}^{7} W_{mk} D_k e^{i\omega_{mk} t},$$  

(10a)

where $W_{mk}$ denotes the matrix elements $\langle m|W|k\rangle$, and $\omega_{mk}$ are defined as

$$\omega_{mk} = \frac{E_m - E_k}{\hbar}.$$  

(10b)

Equation (10a) represents a set of 16 real coupling ordinary differential equations which can be solved numerically, and where $W_{mk}$ are the elements of the matrix

$$(W) = -\frac{\hbar \Omega}{2} \begin{pmatrix}
0 & z^* & 0 & 0 & 0 & 0 & 0 & 0 \\
z & 0 & z^* & 0 & 0 & 0 & 0 & 0 \\
z & 0 & 0 & z^* & 0 & 0 & 0 & 0 \\
0 & z & 0 & 0 & 0 & 0 & 0 & z^* \\
z & 0 & 0 & 0 & z^* & 0 & 0 & 0 \\
z & 0 & 0 & z & 0 & z^* & 0 & 0 \\
z & 0 & 0 & z & 0 & 0 & z^* & 0 \\
0 & z & 0 & z & 0 & z & 0 & 0
\end{pmatrix}.$$  

(10c)

where $z$ is defined as $z = e^{i\omega t}$ and $z^*$ is its complex conjugate.
3. Numerical simulations

To solve (10a) numerically, we shall use similar values for the parameters as [9]. So, in units of $2\pi \times \text{MHz}$, we set the following values:

$$
\omega_0 = 100, \quad \omega_1 = 200, \quad \omega_2 = 400, \quad J = 5, \quad \Omega = 0.1. \quad (11)
$$

The coupling constant $J'$ is chosen to be at least one order of magnitude less than $J$ since in the chain of spins one expects the second neighbour contribution to be at least one order of magnitude weaker than the first neighbour contribution. We consider a digital initial state and superposition initial states,

$$
\Psi_1(0) = |110\rangle, \quad (12a)
$$

and

$$
\Psi(0) = \frac{2}{3\sqrt{8}} |000\rangle + \frac{\sqrt{14}}{3\sqrt{8}} |001\rangle + \frac{1}{3\sqrt{8}} |010\rangle + \frac{\sqrt{17}}{3\sqrt{8}} |011\rangle
$$

$$
+ \frac{3}{4\sqrt{8}} |100\rangle + \frac{\sqrt{23}}{4\sqrt{8}} |101\rangle + \frac{1}{2\sqrt{8}} |110\rangle + \frac{\sqrt{7}}{2\sqrt{8}} |111\rangle, \quad (12b)
$$

to cover all the important aspects of the CNN quantum gate. In all our simulations the total probability, $\sum |C_k(t)|^2$, is kept equal to one within a precision of $10^{-6}$ (note that $|C_k| = |D_k|$). Figure 2 shows the behaviour of $\text{Re} D_6$, $\text{Re} D_7$ and $\text{Im} D_7$ during a $\pi$-pulse ($t = \tau = \pi/\Omega$) for the digital initial state and with $J' = 0.1$. One can see clearly the transition $|110\rangle \rightarrow i|111\rangle$, defining the CCN quantum gate up to a global phase (\pi/2). Figure 3(a) shows the behaviour of the probabilities $|C_k|$ for $k = 0, \ldots, 7$ during a $\pi$-pulse for the superposition initial state and with $J' = 0.1$ and for the superposition initial condition. Figure 3(b) shows the behaviour of the expected value of the $z$-component of the spin, $\langle I_z \rangle_k$, $k = 0, 1, 2$, during a $\pi$-pulse with the initial superposition state and $J' = 0.1$. These expected values are given by

$$
\langle I_z \rangle_k = \frac{1}{2} \sum_{k=0}^{7} (-1)^k |C_k(t)|^2, \quad (13a)
$$
Figure 3. For the superposition initial state and for $J' = 0.1$: (a) probabilities $|C_k(t)|^2$ for $k = 0, \ldots, 7$; (b) expected values (0) $\langle I_0 \rangle$, (1) $\langle I_1 \rangle$ and (2) $\langle I_2 \rangle$.

\[
\langle I_0 \rangle = \frac{1}{2} \{ |C_0|^2 + |C_1|^2 - |C_2|^2 - |C_3|^2 + |C_4|^2 + |C_5|^2 - |C_6|^2 - |C_7|^2 \} \quad (13b)
\]

and

\[
\langle I_2 \rangle = \frac{1}{2} \sum_{k=0}^{3} |C_k|^2 - \sum_{k=4}^{7} |C_k|^2. \quad (13c)
\]

As one could expect, only the spin related to the first qubit (having subindex zero) changes its value at the end of the $\pi$-pulse. The behaviour of the expected values of the $x$ and $y$ components of the spin, $\langle I_x \rangle_k$ and $\langle I_y \rangle_k$ for $k = 0, 1, 2$, is shown in figure 4 for the superposition initial state and for $J' = 0.1$. These expected values are given by

\[
\langle I_0 \rangle = \text{Re}(C_0^* C_0 + C_3^* C_3 + C_5^* C_5 + C_7^* C_7), \quad \langle I_0 \rangle = \text{Im}(\cdots), \quad (14a)
\]

\[
\langle I_1 \rangle = \text{Re}(C_1^* C_0 + C_2^* C_1 + C_4^* C_2 + C_6^* C_3), \quad \langle I_1 \rangle = \text{Im}(\cdots), \quad (14b)
\]

and

\[
\langle I_2 \rangle = \text{Re}(C_2^* C_0 + C_5^* C_1 + C_7^* C_2 + C_3^* C_3), \quad \langle I_2 \rangle = \text{Im}(\cdots). \quad (14c)
\]

The fast oscillations appearing in this behaviour are due to the time dependent phases in equation (8) which have these terms and which are not cancelled out.

For the case $J' = 0$, the resonant frequency for the transition $|110\rangle \leftrightarrow |111\rangle$ and the transition $|010\rangle \leftrightarrow |011\rangle$ coincides and both transitions appear in the dynamics of the system (simultaneous CN and CCN operations). Thus, the question which arises is what is the minimum value of $J'$ which allows us to have a well-defined CCN quantum gate? To answer this question, figures 5(a) and (b) show the behaviour of the CN quantum gate with the resonant frequency of the CCN quantum gate ($\omega = \omega_0 - J - J'$) during a $\pi$-pulse for several $J'$ values. In addition, figures 5(c) and (d) show the fidelity [14], $F = \langle \Psi_{\text{expected}} | \Psi(\tau) \rangle$, associated with CCN quantum gate as a function of $J'/J$. As one can see from these figures, with $J'$ values of even two orders of magnitude lower than $J$, $(J'/J = 0.02)$ we can already have a very well-defined CCN quantum gate. Therefore, it is very likely that a single pulse CCN quantum gate can be implemented in a chain of nuclear spins quantum computer.
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Figure 4. For the superposition initial state and for $J' = 0.1$, expected values of the transversal components of the spin.

Figure 5. For the superposition initial condition. (a) Probability $|C_2|^2$ and (b) probability $|C_3|^2$ for (1) $J' = 0.0$, (2) $J' = 0.02$, (3) $J' = 0.04$, (4) $J' = 0.06$, (5) $J' = 0.08$ and (6) $J' = 0.1$. (c) Real and imaginary parts of the fidelity. (d) Modulus of fidelity.

4. Conclusions and comments

We presented a study of a controlled–controlled-not (CCN) quantum gate implemented in a chain of weakly Ising interacting nuclear spins and with the use of a single $\pi$-pulse. We
studied this gate with digital and superposition initial states and found an expected global phase for its definition,
\[
\hat{\text{CCN}} = |000\rangle\langle000| + |001\rangle\langle001| + |010\rangle\langle010| + |011\rangle\langle011| + |100\rangle\langle100|
\]
\[
+ |101\rangle\langle101| + i|110\rangle\langle110| + i|111\rangle\langle111|.
\] (15)

Using the fidelity parameter, we have seen that the implementation of a CCN quantum gate in the chain of nuclear spins quantum computer is very likely since the coupling constant to second neighbour interaction can be even two orders of magnitude lower than the first neighbour interaction, and still allow a well-defined CCN quantum gate. Since the eigenvalues in (4a) depend on \(J'\), equation (4b), the detuning factor, defined as \(\Delta = (E_p - E_m)/\hbar - \omega\) for the transition \(|p\rangle \leftrightarrow |m\rangle\) (decimal notation), will also depend on \(J'\). Therefore, the normal \(2\pi k\) method used in [8] will have to change correspondingly to be able to suppress non-resonant transitions in multiple-pulse algorithms.

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