On quantum logical gate based on ESR

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Abstracts

In classical computer, there exist inevitable demerits for discussing logical gates. One of the demerits is an irreversibility of logical gates, that is the AND and the OR gates. This property causes to the restriction of computational speed for the classical computer. There are several kind of approaches for avoiding these demerits. One of these approaches is proposed by Feynman [1]. He proved that every logical gates can be contructed by combining with only two reversible gates, i.e., the NOT and the Controlled NOT (CNOT) gates.

By the way, there are several approaches for realizing quantum logical gates. One of those approaches is the study by means of a nuclear magnetic resonance (NMR)[3]. Quantum logical gate based on NMR is performed by controlling the nuclear spin under the additive magnetic fields from the environment. However, it might be difficulty to make the logical gate of NMR using a large number of quantum bits (qubits) because of the weakness of the spin-spin interactions among the nucleiars. Since there are lots of electrons even in one atom, one of the authors proposed the atomic quantum computer, which can treat the interactions among these electrons and nuclear.

In this paper, we discuss the quantum logical gate based on the electron spin resonance (ESR). We contruct the NOT and the CNOT gates by using the quantum channel for the nonrelativistic formulation (Bloch equation) of ESR based on [4], which is connected with the investigation for realization of the effective quantum algorithm [2] of NP complete problem.
1 Quantum channel for NOT gate based on ESR

In this section, we construct the quantum channel for the NOT gate based on ESR.

Let 0, 1 be propositions of false and truth, respectively. The truth table of NOT and Controlled NOT gates are denoted by

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Every quantum logical gates can be constructed by the combinations of NOT and Controlled NOT gates. By means of the quantum channel, we denote these gates based on ESR. First of all, let us consider one particle case.

Let \( \mathcal{H}_s \) be \( \mathbb{C}^2 \) with its canonical basis \( u_+ = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \), \( u_- = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \), \( \mathcal{B}(\mathcal{H}_s) \) be the set of all bounded operators on \( \mathcal{H}_s \) and \( \mathcal{B}(\mathcal{H}_s)_{sa} \equiv \{ A \in \mathcal{B}(\mathcal{H}_s) ; A = A^* \} \), where \( A^* \) is the adjoint of \( A \) defined by \( \langle A^* u, v \rangle = \langle u, Av \rangle \) for any \( u, v \in \mathcal{H}_s \).

\( \mathcal{B}(\mathcal{H}_s)_{sa} \) has the basis \( \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), \( \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \), \( \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \), which are called Pauli spin matrices and \( \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \) is an identity matrix on \( \mathcal{H}_s \). That is, \( \sigma = \{ \sigma_x, \sigma_y, \sigma_z \} \) is an orthogonal basis of \( \mathcal{B}(\mathcal{H}_s)_{sa} \) with the scalar product

\[
\langle \sigma_i, \sigma_j \rangle = \frac{1}{2} \text{tr} \sigma_i \sigma_j, \quad j \in \{ x, y, z \}
\]

and satisfies the multiplication table as follows:
\[ \begin{array}{cccc} \sigma_i \sigma_j & \sigma_x & \sigma_y & \sigma_z \\
\sigma_x & \mathbb{1} & i\sigma_z & -i\sigma_y \\
\sigma_y & -i\sigma_z & \mathbb{1} & i\sigma_x \\
\sigma_z & i\sigma_y & -i\sigma_x & \mathbb{1} \\
\end{array} \]

Let \( \vec{S} = (S_x, S_y, S_z) \) be a spin (angular momentum) operator of electron, where \( S_i = \frac{1}{2}\sigma_i \) is a component of spin operator of electron in the direction of \( i \)-axis \( (i = x, y, z) \). We denote unit vectors of \( x, y, z \) axis by \( \vec{e}_x, \vec{e}_y, \vec{e}_z \) and \( \vec{S} \) is the spin vector given by

\[
\vec{S} = (S_x, S_y, S_z) = S_x \vec{e}_x + S_y \vec{e}_y + S_z \vec{e}_z.
\]

Let us consider two magnetic fields \( \vec{B}_0 \) and \( \vec{B}_1 \). \( \vec{B}_0 \) is a static magnetic field given by

\[
\vec{B}_0 = B_0 \vec{e}_z
\]

in the \( z \) direction and \( \vec{B}_1 \) is a rotating magnetic field given by

\[
\vec{B}_1(t) = B_1(\vec{e}_x \cos \omega t + \vec{e}_y \sin \omega t)
\]

with frequency \( \omega \) in the \( xy \) plain, where \( B_0 \) and \( B_1 \) are certain constants due to the magnetic fields.

If \( \vec{B}(t) \) is a magnetic vector defined by

\[
\vec{B}(t) = \vec{B}_1(t) + \vec{B}_0,
\]

then one has

\[
\frac{d\vec{S}}{dt} = \vec{S} \times \vec{B}(t) = B_1(S_x \cos \omega t + S_y \sin \omega t) + B_0 S_z.
\]

Let \(|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\) and \(|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\) be spin vectors related to spin up and spin down, respectively. Let us take an initial state \( \psi(0) = a_0 |\uparrow\rangle + b_0 |\downarrow\rangle = \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} \) \((a_0, b_0 \in \mathbb{C})\) satisfying \(|a_0|^2 + |b_0|^2 = 1\), then state vector at time \( t \) is denoted by

\[
\psi(t) = a(t) |\uparrow\rangle + b(t) |\downarrow\rangle = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix},
\]

where \( a(t), b(t) \in \mathbb{C} \) are satisfying \(|a(t)|^2 + |b(t)|^2 = 1\).
**Theorem 1** If we start from our spin $|\uparrow\rangle$, i.e., $\vec{S} = \xi \vec{e}_z$ to apply $\vec{B}_1(t)$ for time $t = t_1$ such that $B_1t_1 = \frac{\pi}{2}$ ($\frac{\pi}{2}$ pulse) then our magnet will be in $\vec{S} = \xi \vec{e}_y$ under the condition $\omega = B_1$, where $\xi$ is a certain constant.

**Theorem 2** If we have the eigenvalue equation

$$i \frac{\partial \psi(t)}{\partial t} = -\vec{S} \times \vec{B}(t) \psi(t) = -[B_1(S_x \cos(\omega t) + S_y \sin(\omega t)) + B_0 S_z] \psi(t)$$

when $[S_x, S_y] = iS_z$ is hold and $B_0, B_1, \omega$ are arbitrary constants, then the solution has the form

$$\psi(t) = e^{-i\omega t S_z} e^{iB_1 t(S_x + B_0 S_z)} \psi(0).$$

In particular, we see the **resonance condition**

$$\omega + B_0 = 0,$$

that is,

$$\psi(t) = e^{iB_0 t S_z} e^{itB_1 S_x} \psi(0).$$

Based on the above results, we reconstruct the Not gate based on ESR using by quantum channel.

Let us take $u_+$ and $u_-$ as

$$u_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad u_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Then one can get the following relations:

$$S_x u_+ = \frac{1}{2} u_-,$$

$$S_x u_- = \frac{1}{2} u_+,$$

$$S_z u_+ = \frac{1}{2} u_+,$$

$$S_z u_- = -\frac{1}{2} u_-.$$
Theorem 3 For the initial state vector $\psi(0) = a_0 u_+ + b_0 u_- = \begin{pmatrix} a_0 \\ b_0 \end{pmatrix}$, $(a_0, b_0 \in \mathbb{C})$, one can obtain by using the theorem 2

$$
\psi(t) = \left[ a_0 \cos \left( \frac{B_1 t}{2} \right) + i b_0 \sin \left( \frac{B_1 t}{2} \right) \right] \exp \left( \frac{i B_0 t}{2} \right) u_+ \\
+ \left[ b_0 \cos \left( \frac{B_1 t}{2} \right) + i a_0 \sin \left( \frac{B_1 t}{2} \right) \right] \exp \left( \frac{-i B_0 t}{2} \right) u_-.
$$

For example, we take $a_0 = 1, b_0 = 0$, that is, the state vectors at time 0 and $t$ are

$$
\psi(0) = u_+, \\
\psi(t) = \cos \left( \frac{B_1 t}{2} \right) \exp \left( \frac{i B_0 t}{2} \right) u_+ + i \sin \left( \frac{B_1 t}{2} \right) \exp \left( \frac{-i B_0 t}{2} \right) u_-.
$$

If we take $t = t_1$ such that $\frac{B_0 t_1}{2} = \frac{B_1 t_1}{2} = \frac{\pi}{2}$ ($\pi$ pulse) then

$$
\psi(t_1) = u_-.
$$

Indeed we take $a_0 = 0, b_0 = 1$, that is, the state vectors at time 0 and $t$ are

$$
\psi(0) = u_-, \\
\psi(t) = i \sin \left( \frac{B_1 t}{2} \right) \exp \left( \frac{i B_0 t}{2} \right) u_+ + \cos \left( \frac{B_1 t}{2} \right) \exp \left( \frac{-i B_0 t}{2} \right) u_-.
$$

If we take $t = t_1$ such that $\frac{B_0 t_1}{2} = \frac{B_1 t_1}{2} = \frac{\pi}{2}$ ($\pi$ pulse) then

$$
\psi(t_1) = -u_+.
$$

It means that this gate is performed as the NOT gate based on ESR.

Let $U_{NOT}(t) \equiv e^{i B_0 t S_z} e^{i B_1 t S_x}$ be a unitary operator expressing the NOT gate based on ESR. Quantum channel denoting the NOT gate based on ESR is defined by

$$
\Lambda_{NOT(t_1)}^* (\bullet) \equiv U_{NOT}(t_1) (\bullet) U_{NOT}(t_1)^*.
$$

For the initial state $|\psi(0)\rangle \langle \psi(0)|$ at time 0, the output state of $\Lambda_{NOT(t_1)}^*$ is obtained by

$$
\Lambda_{NOT(t_1)}^* (|\psi(0)\rangle \langle \psi(0)|) = |\psi(t_1)\rangle \langle \psi(t_1)|.
$$
Thus we have the complete truth table of the NOT gate based on ESR such as

\[
\begin{array}{c|c}
I_{\text{NOT}} & O_{\text{NOT}} \\
\hline
1 & 0 \\
0 & 1 \\
\end{array}
\]

2 Quantum channel for CNOT gate based on ESR

In this section, we introduce the quantum channel for the CNOT gate based on ESR.

Let us consider \( N \) particle systems to treat the Controlled Not gate.

Let \( \vec{e}_1, \vec{e}_2, \vec{e}_3 \) be unit vectors of \( x, y, z \) axis, respectively, and let \( \vec{S}^{(1)}, \ldots, \vec{S}^{(N)} \) be spin vectors of \( N \) electrons such as

\[
\vec{S}^{(i)} = \left( S_1^{(i)}, S_2^{(i)}, S_3^{(i)} \right) = S_1^{(i)} \vec{e}_1 + S_2^{(i)} \vec{e}_2 + S_3^{(i)} \vec{e}_3.
\]

The spin operators satisfy the following commutation relations

\[
\left[ S_\alpha^{(p)}, S_\beta^{(q)} \right] = i \delta_{pq} \sum_{\gamma=1}^{3} \epsilon_{\alpha\beta\gamma} S_\gamma^{(q)},
\]

where \( \epsilon_{\alpha\beta\gamma} = \left\{ \begin{array}{ll} +1 & \text{and} \delta_{pq} \text{ is a certain constant.} \\
-1 & \end{array} \right. \)

Let us consider a Hamilnotian operator for \( N \) particle systems given by

\[
H_{(N)} \equiv B_3 \left( \sum_{i=1}^{N} S_3^{(i)} \right) + B_1 \left( \sum_{i=1}^{N} S_1^{(i)} \right) f(t) + \sum_{i,j=1}^{N} J_{ij} S_3^{(i)} \otimes \overline{S}_3^{(j)},
\]

where \( f(t) \) is a certain function, for example \( f(t) = \cos \omega t \) and \( J_{ij} \) is a coupling constant with respect to \( i \)-th spin and \( j \)-th spin.

\( S_k^{(i)} \) is embedding \( S_k \) into \( i \)-th position of \( N \) tensor product.

\[
S_k^{(i)} = I \otimes \cdots \otimes S_k \otimes \cdots \otimes I, \quad (k = 1, 2, 3).
\]
Let us take a Hamiltonian $H_{(N)}$ as an Ising type interaction, that is
\[ H_{(N)} \equiv B_3 \left( \sum_{i=1}^{N} S_3^{(i)} \right) + \sum_{i,j=1}^{N} J_{ij} S_3^{(i)} \otimes \overline{S}_3^{(j)}. \]

If $N = 2$ then one can denote
\[ H_{(2)} = B_3 \left( S_3 \otimes I + I \otimes \tilde{S}_3 \right) + J \left( S_3 \otimes \tilde{S}_3 \right) + B_0 \left( I \otimes I \right), \]
where $B_0$, $B_3$ and $J$ are determined by a certain phase parameter $\omega$. Then we have
\[
\begin{align*}
e^{-2i\omega t(S_3 \otimes S_3)} &= \sum_{n=0}^{\infty} \frac{(i)^n (-2\omega t)^n}{n!} \left( S_3 \otimes \tilde{S}_3 \right)^n \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n (-2\omega t)^{2n}}{2n!} \left( S_3 \otimes \tilde{S}_3 \right)^{2n} \\
&\quad + i \sum_{n=0}^{\infty} \frac{(-1)^n (-2\omega t)^{2n+1}}{(2n + 1)!} \left( S_3 \otimes \tilde{S}_3 \right)^{2n+1} \\
&= \sum_{n=0}^{\infty} \frac{(-\omega t)^{2n}}{2n!} \left( I \otimes I \right) + 4i \sum_{n=0}^{\infty} \frac{(-\omega t)^{2n+1}}{(2n + 1)!} \left( S_3 \otimes \tilde{S}_3 \right) \\
&= \cos \left( \frac{\omega t}{2} \right) \left( I \otimes I \right) - 4i \sin \left( \frac{\omega t}{2} \right) \left( S_3 \otimes \tilde{S}_3 \right).
\end{align*}
\]
Indeed one can obtain
\[
\begin{align*}
e^{i\omega t(I \otimes S_3)} &= \cos \left( \frac{\omega t}{2} \right) \left( I \otimes I \right) + 2i \sin \left( \frac{\omega t}{2} \right) \left( I \otimes \tilde{S}_3 \right), \\
e^{i\omega t(S_3 \otimes I)} &= \cos \left( \frac{\omega t}{2} \right) \left( I \otimes I \right) + 2i \sin \left( \frac{\omega t}{2} \right) \left( S_3 \otimes I \right).
\end{align*}
\]
Let us take $u_+, u_-, v_+, v_-$ as
\[
\begin{align*}
u_+ \otimes v_+ &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, & u_+ \otimes v_- &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},
\end{align*}
\]
Then one has
\begin{align*}
S_1 u_+ &= +\frac{1}{2} u_-, S_1 u_- = +\frac{1}{2} v_+, \\
\tilde{S}_1 v_+ &= +\frac{1}{2} v_-, \tilde{S}_1 v_- = +\frac{1}{2} v_+, \\
S_3 u_+ &= +\frac{1}{2} u_+, S_3 u_- = -\frac{1}{2} u_-, \\
\tilde{S}_3 v_+ &= +\frac{1}{2} v_+, \tilde{S}_3 v_- = -\frac{1}{2} v_-,
\end{align*}

Let \( \psi(0) \) be an initial state vector given by
\[
\psi(0) = a_0 u_+ \otimes v_+ + b_0 u_- \otimes v_+ + c_0 u_+ \otimes v_- + d_0 u_- \otimes v_- = \begin{pmatrix} a_0 \\ b_0 \\ c_0 \\ d_0 \end{pmatrix}, \quad (a_0, b_0, c_0, d_0 \in \mathbb{C}).
\]

For the initial state vector \( \psi(0) \), if \( J = 2\omega, B_3 = -\omega \) and \( B_0 = \frac{1}{2}\omega \) are hold, then the state vector at time \( t \) is expressed by
\[
\Psi(t) = e^{i\omega t(S_3 \otimes I)} e^{i\omega t(I \otimes \tilde{S}_3)} e^{-2i\omega t(S_3 \otimes \tilde{S}_3)} e^{-\frac{1}{2}i\omega t(I \otimes I)} \psi(0).
\]

**Theorem 4** For the initial state vector \( \psi(0) \), one can obtain
\[
\psi(t) = e^{i\omega t(S_3 \otimes I)} e^{i\omega t(I \otimes \tilde{S}_3)} e^{-2i\omega t(S_3 \otimes \tilde{S}_3)} e^{-\frac{1}{2}i\omega t(I \otimes I)} \psi(0)
= (a_0 u_+ \otimes v_+ + b_0 u_- \otimes v_+ + c_0 u_+ \otimes v_-) + d_0 \exp(-2i\omega t) u_- \otimes v_-.
\]

For example, if we take \( a_0 = 1 \) or \( b_0 = 1 \) or \( c_0 = 1 \), then we have \( \psi(t) = \psi(0) \). Let us take \( d_0 = 1 \), that is
\[
\psi(0) = u_- \otimes v_-.
\]
the state vector at time $t$ is obtained by
\[ \psi(t) = \exp(-2i\omega t) u_- \otimes v_- . \]
If we take $t = t_1$ such that $2\omega t = \pi$ (\(\frac{\pi}{2}\) pulse) then one has
\[ \psi(t_1) = -u_- \otimes v_- . \]

Therefore one can denote the matrix form $U_\Phi(t_1)$ of $e^{i\omega t_1(S_3 \otimes I)} e^{i\omega t_1(I \otimes \overline{S}_3)} \times e^{-2i\omega t_1(S_3 \otimes \overline{S}_3)} e^{-\frac{1}{2}i\omega t_1(I \otimes I)}$ by
\[ U_\Phi(t_1) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} . \]

Next we construct a unitary operator $U_H(t)$ related to a Hadamard transformation based on ESR. Let us define $U_H(t)$ by
\[ U_H(t) = e^{-i\omega_2 t(I \otimes \overline{S}_2)} , \]
where $\omega_2$ is a certain phase parameter. Then we have
\[ e^{-i\omega_2 t(I \otimes \overline{S}_2)} = \cos \left( \frac{\omega_2 t}{2} \right) (I \otimes I) - 2i \sin \left( \frac{\omega_2 t}{2} \right) (I \otimes \overline{S}_2) . \]

For the intital state vector $\psi(0)$, the state vector at time $t$ is expressed by
\[ \psi(t) = U_H(t) \psi(0) = e^{-i\omega_2 t(I \otimes \overline{S}_2)} \psi(0) . \]

**Theorem 5** For the initial state vector $\psi(0) = a_0 u_+ \otimes v_+ + b_0 u_- \otimes v_+ + c_0 u_+ \otimes v_- + d_0 u_- \otimes v_-$, \((a_0, b_0, c_0, d_0 \in \mathbb{C})\), one can obtain
\[ \psi(t) = e^{-i\omega_2 t(I \otimes \overline{S}_2)} \psi(0) = a_0 u_+ \otimes \left( \cos \left( \frac{\omega_2 t}{2} \right) v_+ + \sin \left( \frac{\omega_2 t}{2} \right) v_- \right) \\
+ b_0 u_- \otimes \left( \cos \left( \frac{\omega_2 t}{2} \right) v_+ + \sin \left( \frac{\omega_2 t}{2} \right) v_- \right) \\
+ c_0 u_+ \otimes \left( -\sin \left( \frac{\omega_2 t}{2} \right) v_+ + \cos \left( \frac{\omega_2 t}{2} \right) v_- \right) \\
+ d_0 u_- \otimes \left( -\sin \left( \frac{\omega_2 t}{2} \right) v_+ + \cos \left( \frac{\omega_2 t}{2} \right) v_- \right) . \]
If we take $t = t_2$ such that $\frac{\omega_2 t}{2} = \frac{\pi}{4}$ ($\frac{\pi}{2}$ pulse), then one has

$$\psi (t_2) = (a_0 u_+ + b_0 u_-) \otimes \frac{1}{\sqrt{2}} (v_+ + v_-) + (c_0 u_+ + d_0 u_-) \otimes \frac{1}{\sqrt{2}} (-v_+ + v_-).$$

Then one can denote the matrix form $U_H (t_2)$ of $e^{-i\omega_2 t_2 (I \otimes \overline{s}_2)}$ by

$$U_H (t_2) = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \otimes \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array} \right).$$

Thus unitary operator $U_{CNOT} (t_1 + 2t_2)$ related to the CNOT gate can be reconstructed by the convection of $U_{\Phi} (t_1)$ and $U_H (t_2)$ as

$$U_{CNOT} (t_1 + 2t_2) = U_H (t_2)^* U_{\Phi} (t_1) U_H (t_2)$$

$$= e^{i\omega_2 t_2 (I \otimes \overline{s}_2)} e^{i\omega t_1 (S_3 \otimes I)} e^{i\omega t_1 (I \otimes \overline{s}_3)} \times$$

$$\times e^{-2i\omega t_1 (S_3 \otimes \overline{s}_3)} e^{-\frac{1}{2}i\omega t_1 (I \otimes I)} e^{-i\omega_2 t_2 (I \otimes \overline{s}_2)}$$

and the matrix form of $U_{CNOT} (t_1 + 2t_2)$ is obtained by

$$U_{CNOT} (t_1 + 2t_2) = \left( \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right).$$

It means that this unitary operator $U_{CNOT} (t_1 + 2t_2)$ is performed as CNOT (Controlled NOT) gate based on ESR. Quantum channel denoting the CNOT gate based on ESR is defined by

$$\Lambda^*_{CNOT(t_1+2t_2)} (\bullet) \equiv U_{CNOT} (t_1 + 2t_2) (\bullet) U_{CNOT}^* (t_1 + 2t_2).$$

For the initial state $|\psi (0)\rangle \langle \psi (0)|$ at time 0, the output state of $\Lambda^*_{CNOT(t_1+2t_2)}$ is obtained by

$$\Lambda^*_{CNOT(t_1+2t_2)} (|\psi (0)\rangle \langle \psi (0)|) = |\psi (t_1 + 2t_2)\rangle \langle \psi (t_1 + 2t_2)|.$$

Thus we have the complete truth table of the CNOT gate based on ESR such as

$$u_+ \leftrightarrow 1$$

$$u_- \leftrightarrow 0$$

$$v_+ \leftrightarrow 1$$

$$v_- \leftrightarrow 0$$
In order to make our discussion more rigorously, we will discuss the quantum channel for NOT and CNOT gates under the Dirac formulation (fine (Relativistic) formulation) of electron and under the Hyperfine formulation including the interaction between electrons and nuclear in our further study of ESR.

**References**


