Nuclear Magnetic Resonance Based Quantum computer

Abstract

NRM qubit calculations.

Index Terms

NRM,qubit, quantum computer

Contents

I. Inroduction

A spin 1/2 nucleus or an electron placed in a magnetic field of strength B can be described by the Hamiltonian

$$H = -\frac{\hbar w_0}{2}\sigma_z, \tag{1}$$

where σ_z is the 3^{rd} Pauli matrix and $w_0 = \mu B$, μ being the magnetic dipole moment of the particle. In this representation the eigenstates can be written explicitly as

$$|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \ |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{2}$$

Let us now introduce a magnetic field in the x direction,

$$\vec{B_1} = -B_1 \cos(\omega_{rf} t - \phi)\hat{x}. \tag{3}$$

The full Hamiltonian becomes

$$H = -\frac{\hbar w_0}{2}\sigma_z + 2\hbar w_1 cos(\omega_{rf} t - \phi)\sigma_x, \tag{4}$$

where $w_1 = \gamma B_1/2$. Here we assume that $w_0 \ll w_1$. The Schrodinger Equation reads

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \tag{5}$$

Since the Hamiltonian is time dependent, it is convenient to describe the problem in a rotating frame such that the Hamiltonian in that frame becomes time independent. Let us define

$$|\psi(t)\rangle = U_R(t)|\psi_R(t)\rangle, \tag{6}$$

where

$$U_R(t) = e^{-i\frac{w}{2}t\sigma_z}. \tag{7}$$

Inserting Eq. (6) in to Eq. (5) yields

$$i\frac{\partial}{\partial t}|\psi_R(t)\rangle = \left(U_R H(t) U_R^\dagger - i\hbar U_R \frac{d}{dt} U_R^\dagger\right)|\psi_R(t)\rangle, \tag{8}$$

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which shows that the Hamiltonian in the rotating frame is

$$\tilde{H} = U_R H U_R^\dagger - i\hbar U_R \frac{d}{dt} U_R^\dagger, \tag{9}$$

and we also used

$$\frac{d}{dt} U_R U_R^\dagger = -U_R \frac{d}{dt} U_R^\dagger. \tag{10}$$

We can calculate Eq. (9) explicitly as

$$\begin{aligned} \tilde{H} &= U_R H U_R^\dagger - i\hbar U_R \frac{d}{dt} U_R^\dagger \\ &= -(w - w_1)\sigma_z/2 \\ &+ w_1 \cos(w_{rf}t - \phi) e^{-iwt\sigma_z t/2} \sigma_x e^{iwt\sigma_z t/2}. \end{aligned} \tag{11}$$

We can use the following property of the Pauli matrices

$$e^{-iwt\sigma_z t/2} \sigma_x e^{iwt\sigma_z t/2} = \sigma_x \cos(wt) + \sigma_y \sin(wt). \tag{12}$$

Inserting this into Eq. (11) we get,

$$\begin{aligned} \tilde{H} &= \begin{pmatrix} -\frac{w-w_1}{2} & w_1 e^{-iwt}\cos(w_{rf}t - \phi) \\ w_1 e^{iwt}\cos(w_{rf}t - \phi) & \frac{w-w_1}{2} \end{pmatrix} \\ &= \frac{w_1}{2} \begin{pmatrix} -\frac{w-w_1}{w_1} & e^{-i(\Delta t+\phi)} e^{-i(\Sigma t - \phi)} \\ e^{i(\Delta t+\phi)} + e^{i(\Sigma t - \phi)} & \frac{w-w_1}{w_1} \end{pmatrix} \end{aligned} \tag{13}$$

where we define $\Sigma = w + w_{rf}$ and $\Delta = w - w_{rf}$. It is important to note that w_{rf} is the frequency of the magnetic field, therefore we can choose it such that $w_{rf} = w_0$. In this case $\Sigma = 2w_{rf}$ and $\Delta = 0$. Furthermore the terms with Σ are rapidly oscillating and their average becomes zero over the time scale $1/w_1$, which is the time scale for rotations. This approximation is called the **rotating wave approximation**. In this limit $\tilde{H}$ becomes time independent,and reads

$$\tilde{H} = \frac{\hbar\omega_1}{2}(\cos\phi\sigma_x + \sin\phi\sigma_y) = \hbar\omega_1 \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \tag{14}$$

This completes the simplification of the Hamiltonian. We now discuss how this Hamiltonian can implement single qubit operations.

II. Single qubit operations

It is obvious that Hamiltonian in Eq. (14) can easily generate rotations around x and y-axis. If one chooses $\phi = 0$ or $\phi = \pi$, the time development operator reads

$$U(t) = e^{-i\tilde{H}t/\hbar} = e^{\mp i \frac{w_1 t}{2} \sigma_x}, \tag{15}$$

which clearly generates rotations around $\pm x$-axis. Similarly if one chooses $\phi = \pm\pi/2$, the time development operator reads

$$U(t) = e^{-i\tilde{H}t/\hbar} = e^{\mp i \frac{w_1 t}{2} \sigma_y}, \tag{16}$$

which generates rotations around $\pm y$-axis. Although Eq. (14) lacks σ_z, the rotations around z-axis can be generated as a series of rotations around x and y axes. This follows from the identity

$$e^{-i\alpha\sigma_z/2} = e^{-i\frac{\pi}{2}\sigma_x/2} e^{-i\alpha\sigma_y/2} e^{-i\frac{\pi}{2}\sigma_x/2}. \tag{17}$$

Therefore we conclude that the nuclear spin can be rotated to any point in the Bloch Sphere.

III. Two-qubit operations

Now we need to describe two qubits using the Hamiltonian of individual qubits and their interactions. Let split the Hamiltonian into three pieces:

$$H = H_0 + H_{rf,1} + H_{rf,2}. \tag{18}$$

The first term is the time independent part that includes interaction of the qubits with the external magnetic field along z-axis and the inter-qubit interaction:

$$H_0 = -w_{0,1} I_z \otimes I - w_{0,2} I \otimes I_z + J \sum_k I_k \otimes I_k, \tag{19}$$

where the last term is the interaction of the magnetic dipoles of the qubits. The second and the third terms in Eq. (18) are the interactions of the qubits with the time varying control field along the x-axis,

$$H_{rf,1} = 2\hbar w_{1,1} cos(\omega_{rf,1} t - \phi_1)(I_x \otimes I + g I \otimes I_x), \tag{20}$$

and

$$H_{rf,2} = 2\hbar w_{1,2} cos(\omega_{rf,2} t - \phi_2)(g^{-1} I_x \otimes I + I \otimes I_x), \tag{21}$$

where

$$2w_{1,i} = \gamma_i B_{1,i} \quad and \quad g = \gamma_2/\gamma_1. \tag{22}$$

We will employ the same trick of transforming into the rotating frame using the following operator:

$$U_R(t) = e^{-iw_{0,1} I_z t} \otimes e^{-iw_{0,2} I_z t} \tag{23}$$

In this frame, the transformed Hamiltonian reads

$$\begin{aligned} \tilde{H} = J I_z \otimes I_z \quad &+ \quad \hbar w_{1,1}[cos\phi_1 I_x \otimes I + \sin\phi_1 I_y \otimes I] \\ &+ \quad \hbar w_{1,2}[cos\phi_2 I \otimes I_x + \sin\phi_2 I \otimes I_y], \end{aligned} \tag{24}$$

which is basically the final form of the Hamiltonian. Keep in mind that $w_{1,i}$ is tied to the external field along the x-axis, which we can turn on and off. When that control field is turned off, the dynamics of the qubits is simply driven by the interaction term 1; therefore, the time evolution operator corresponding to the Hamiltonian in Eq. (24) simplifies to:

$$U_R(t) = e^{-iJ I_z \otimes I_z t} = \begin{pmatrix} e^{-i\frac{Jt}{4}} & 0 & 0 & 0 \\ 0 & e^{i\frac{Jt}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{Jt}{4}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{Jt}{4}} \end{pmatrix} \tag{25}$$

Before we proceed, let's take a look at the values of these frequencies for a couple of molecules:

molecule	$w_{0,1}$	$w_{0,2}$	J
Chloroform	500 Mhz	100 Mhz	200 Hz
Cytosine	500 Mhz	500 Mhz	7.1 Hz

Note how small are the frequencies corresponding to the qubit interaction term J. This implies that the time evolution operator in Eq. (25) is very slow. For Cytosine it will take 1/7.1 seconds to complete a full period!

If we let the system evolve for a period of time $\tau = \pi/J$, we get

$$U_R(\frac{\pi}{J}) = e^{-i\pi I_z \otimes I_z} = \begin{pmatrix} e^{-i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \end{pmatrix}, \tag{26}$$

which is a particularly useful transformation matrix. Let's do a very special series of transformations as follows:

$$Z_1 \bar{Z}_2 X_2 U_R(\frac{\pi}{J}) Y_2 = e^{-i\frac{\pi}{4}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{27}$$

The operator in Eq. (27) is the Holy Grail of quantum operations: it is U_{CNOT}, which flips the second qubit only if the first qubit is 1. It is necessary and sufficient to create all possible 2-qubit operations. This completes the derivation that the NRM computer can create any possible single qubit or two-qubit operations. And it is rather straight forward to extend this to multi-qubit case by simply generalizing Eq. (24) as follows:

$$\tilde{H} = \sum_{i=1}^{n-1} J_{i,i+1} I_{z,i} \otimes I_{z,i+1} + \sum_{i=1}^{n} \hbar w_{1,i} [cos\phi_i I_x + \sin\phi_i I_y] \tag{28}$$

which shows that it is possible to execute U_{CNOT} operations for any qubit pairs.

1 Keep in mind that we are in the rotating frame and the effect of the external field along z-axis is taken care of.