

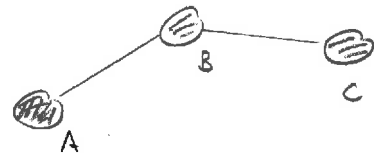
Term paper:

Final presentation: ~~Tues 11~~ Tues 11 Dec 1-3pm  
(about 15 minutes each)

Gates for spin-1/2 qubits

We consider a molecule consisting of distinct spin-1/2 nuclei, each of which represents a distinct qubit. These are placed in a constant magnetic field

$$\vec{B} = B_0 \hat{z}$$



The resulting Hamiltonian for any single spin is:

$$\hat{H} = \frac{\hbar \omega_0}{2} \hat{\sigma}_z$$

where  $\omega_0$  is proportional to  $B_0$  and other quantities that only depend on the nucleus and its immediate environment. It follows that if the system is allowed to evolve for time  $t$  then the unitary evolution operator is

$$\hat{U}(t) = e^{-i\omega_0 t \hat{\sigma}_z / 2}$$

This is a rotation about the z-axis through angle  $\omega t$ .

Thus

An arbitrary rotation about the z-axis can be attained by letting the system evolve for the appropriate time  $t$  under  $\vec{B} = B_0 \hat{z}$

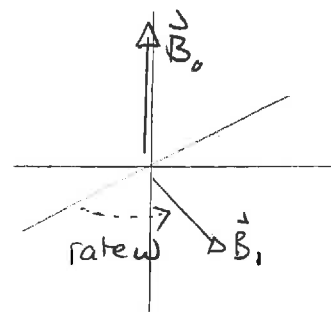
To produce a rotation about a perpendicular axis we supply an additional rotating magnetic field

$$\vec{B}_1 = B_1 [\cos \omega t \hat{x} + \sin \omega t \hat{y}]$$

and let the system evolve under  $\vec{B} = \vec{B}_0 + \vec{B}_1$ .

By moving to the rotating frame we can eventually show that the unitary evolution operator is

$$\hat{U}(t) = e^{-i\omega t \hat{\sigma}_z / 2} e^{-i \hat{H}_{\text{rot}} t / \hbar}$$



where

$$\hat{H}_{\text{rot}} = \frac{\hbar}{2} (\omega_0 - \omega) \hat{\sigma}_z + \frac{\hbar \omega_1}{2} \hat{\sigma}_x$$

and  $\omega_1$  is proportional to  $B_1$ . So

$\omega_0 \rightsquigarrow$  strength of  $\vec{B}_0$

$\omega_1 \rightsquigarrow$  " "  $\vec{B}_1$

$\omega \rightsquigarrow$  rate at which  $\vec{B}_1$  rotates

Then the rightmost term in  $\hat{U}(t)$  is:

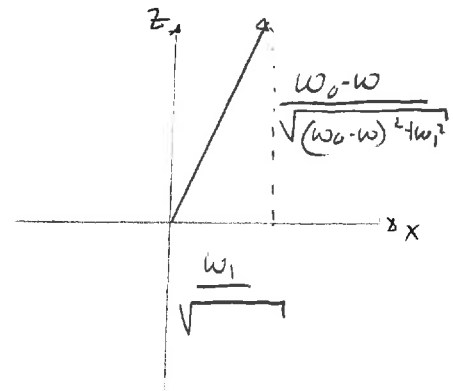
$$e^{-i[(\omega_0 - \omega)\hat{\sigma}_z + \omega_1\hat{\sigma}_x]t/2}$$

which is a rotation about an axis in the x-z plane. Specifically

$$\text{with } (\omega_0 - \omega)\hat{\sigma}_z + \omega_1\hat{\sigma}_x = \left[ (\omega_0 - \omega)\hat{\sigma}_z + \omega_1\hat{\sigma}_x \right] \frac{\sqrt{(\omega_0 - \omega)^2 + \omega_1^2}}{\sqrt{(\omega_0 - \omega)^2 + \omega_1^2}}$$

we see that it is a rotation about the illustrated unit vector through angle  $\sqrt{(\omega_0 - \omega)^2 + \omega_1^2} t$ .

We can therefore engineer a rotation about  $\hat{x}$  by adjusting  $\omega = \omega_0$ .



Thus we get

$$\hat{U}(t) = \underbrace{e^{-i\omega_0 t \hat{\sigma}_z / 2}}_{\text{rotation about } z \text{ through } \omega_0 t} \underbrace{e^{-i\omega_1 t \hat{\sigma}_x / 2}}_{\text{rotation about } x \text{ through } \omega_1 t}$$

rotation about  $z$  through  $\omega_0 t$       rotation about  $x$  through  $\omega_1 t$

So we can do a rotation about  $\hat{x}$  by:

Apply a rotating magnetic field with rotation rate  $\omega = \omega_0$ .

Then

Run rotating field for time  $t$

→

Turn rotating field off and let spin evolve under  $\vec{B}_0$  only for time  $t'$  s.t.

$$\omega_0(t+t') = 2\pi$$

Rot about  $x$  angle  $\omega_1 t$  + Rot about  $z$  angle  $\omega_0 t$

+

Rot about  $z$  angle  $\omega_0 t'$

≡ Rot about  $x$  angle  $\omega_1 t$

Thus we can get:

Rotation about  $\hat{z}$   $\leadsto$  evolve under  $\vec{B}_0$  only

Rotation about  $\hat{x}$   $\leadsto$  evolve under rotating magnetic field  $\vec{B}$ , with frequency  $\omega = \omega_0$  and also under just  $\vec{B}_0$

This allows us to construct arbitrary rotations about  $\hat{x}$  and  $\hat{z}$  and therefore any rotation about any axis. Thus we can attain any single qubit unitary in this way.

## Two qubit gates

Recall that we need two qubit gates between arbitrary pairs of qubits. If we can generate a CNOT, then we can generate any two qubit gate. So we focus on generating a CNOT. We will

- 1) first show how to construct a CNOT from a controlled- $Z$
- 2) second show how to construct a controlled- $Z$  using a specific interaction between two spins.

## 1 CNOT gates from controlled-Z gates

Recall that a CNOT gate can be represented as

$$\hat{C}_{\hat{\sigma}_x} = |0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_x.$$

A controlled-Z can be represented as

$$\hat{C}_{\hat{\sigma}_z} = |0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_z.$$

- Represent each of these in terms of matrices in the computational basis.
- Show how to construct the CNOT using a controlled-Z and single qubit operations.

Answer: a)  $|0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_x$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{C}_{\hat{\sigma}_x} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Then  $|0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_z$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

$$\Rightarrow \hat{C}_{\sigma_z} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

b) We need a unitary  $\hat{U}$  s.t.  $\hat{U}\hat{U} = \hat{I}$  and  $\hat{U}\hat{\sigma}_z\hat{U} = \hat{\sigma}_x$

$$\begin{aligned} \text{Then } (\hat{I} \otimes \hat{U})(\hat{C}_{\sigma_z})(\hat{I} \otimes \hat{U}) &= |0\rangle\langle 0| \otimes \hat{U}\hat{U} + |1\rangle\langle 1| \otimes \hat{U}\hat{\sigma}_z\hat{U} \\ &= |0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_x \end{aligned}$$

Clearly  $\hat{H}$  works. So



The way in which a two-qubit gate can be constructed requires a coupling between two spins. A specific example of this is the "J coupling" which results from inter-band interactions. The

J-coupling Hamiltonian is

$$\hat{H}_J = \frac{\hbar\pi}{2} J \hat{\sigma}_z \otimes \hat{\sigma}_z$$

We can then explore evolution under this for specified durations of time in conjunction with single qubit gates.

## 2 Evolution under $J$ -coupling

Consider the  $J$  coupling Hamiltonian as presented in lecture.

a) Determine a matrix expression for

$$\hat{U}(t) = e^{-i\hat{H}Jt/\hbar}$$

b) Evaluate the expression for  $t = 1/2J$ .

c) Evaluate the expression for  $t = 1/J$ .

d) Consider  $\hat{U}(1/2J)$  and suggest two single bit rotations, each about the  $z$  axis such that the result is the controlled- $Z$  gate.

Answer: a)  $\hat{H} = \frac{\hbar \pi J}{2} \hat{\sigma}_z \otimes \hat{\sigma}_z$

$$\begin{aligned} \hat{U}(t) &= e^{-i \frac{\pi J t}{2} \hat{\sigma}_z \otimes \hat{\sigma}_z} \\ &= \hat{I} - i \frac{\pi J t}{2} (\hat{\sigma}_z \otimes \hat{\sigma}_z) + \frac{1}{2!} \left( -i \frac{\pi J t}{2} \right) \underbrace{(\hat{\sigma}_z \otimes \hat{\sigma}_z)^2}_{=\hat{I}} + \dots \end{aligned}$$

$$= \hat{I} \cos\left(\frac{\pi J t}{2}\right) - i \hat{\sigma}_z \otimes \hat{\sigma}_z \sin\left(\frac{\pi J t}{2}\right)$$

$$= \cos\frac{\pi J t}{2} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} - i \sin\left(\frac{\pi J t}{2}\right) \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i\pi J t/2} & 0 & 0 & 0 \\ 0 & e^{i\pi J t/2} & 0 & 0 \\ 0 & 0 & e^{i\pi J t/2} & 0 \\ 0 & 0 & 0 & e^{-i\pi J t/2} \end{pmatrix}$$



$$b) \quad \hat{U}(\frac{1}{2}\pi) = \begin{pmatrix} e^{-i\pi/4} & & & \\ & e^{i\pi/4} & & \\ & & e^{i\pi/4} & \\ & & & e^{-i\pi/4} \end{pmatrix} = e^{-i\pi/4} \begin{pmatrix} 1 & & & \\ & e^{i\pi/2} & & \\ & & e^{i\pi/2} & \\ & & & 1 \end{pmatrix}$$

$$c) \quad \hat{U}(\frac{1}{3}\pi) = -i \hat{\sigma}_z \otimes \hat{\sigma}_z = -i \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix}$$

d) Consider a rotation on the left qubit through angle  $\alpha$  and on right by angle  $\beta$ . Then these correspond to

$$\hat{U}_{rot} = e^{-i\alpha\hat{\sigma}_z/2} \otimes e^{-i\beta\hat{\sigma}_z/2}$$

$$= \begin{pmatrix} e^{-i\alpha/2} & 0 \\ 0 & e^{i\alpha/2} \end{pmatrix} \otimes \begin{pmatrix} e^{-i\beta/2} & 0 \\ 0 & e^{i\beta/2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i(\alpha+\beta)/2} & & & \\ & e^{-i(\alpha-\beta)/2} & & \\ & & e^{-i(\beta-\alpha)/2} & \\ & & & e^{-i(-\alpha-\beta)/2} \end{pmatrix} = e^{-i(\alpha+\beta)/2} \begin{pmatrix} 1 & & & \\ & e^{i\beta} & & \\ & & e^{i\alpha} & \\ & & & e^{i(\alpha+\beta)} \end{pmatrix}$$

Now

$$\hat{U}_{1st} \hat{U} \left( \frac{1}{2J} \right) = e^{i(\alpha+\beta)/2} \begin{pmatrix} 1 & & & \\ & e^{i\beta} & & \\ & & e^{i\alpha} & \\ & & & e^{i(\alpha+\beta)} \end{pmatrix} \begin{pmatrix} 1 & & & \\ & e^{i\pi/2} & & \\ & & e^{i\pi/2} & \\ & & & -1 \end{pmatrix}$$
$$= \underbrace{e^{i(\alpha+\beta)/2}}_{\text{global phase}} \begin{pmatrix} 1 & & & \\ & e^{i(\beta+\pi/2)} & & \\ & & e^{i(\alpha+\pi/2)} & \\ & & & e^{i(\alpha+\beta)} \end{pmatrix}$$

If  $\alpha = \beta = 3\pi/2$  then

$$e^{i(\beta+\pi/2)} = e^{i2\pi} = 1$$
$$e^{i(\alpha+\pi/2)} = e^{i2\pi} = 1$$
$$e^{i(\alpha+\beta)} = e^{i3\pi} = -1$$

So we have constructed the C-Z gate  $\square$

Thus, to construct the controlled-X gate, we can evolve the pair of spins under the J-coupling followed by assorted single bit gates