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# Implementation of multiqubit gates Case of NMR

Introduction to Quantum Computing

**Kenneth MAUSSANG**

Université de Montpellier

2022 – 2023

# Implementation of multiqubit gates - Case of NMR

- 1 Implementation of a C-NOT gate
- 2 Example with NMR quantum computing
- 3 Molecules for quantum computing based on NMR techniques

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- 1 Implementation of a C-NOT gate
  - Ising interaction
  - Two-qubit unitary evolution
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# 1.1. Ising interaction

Let consider an ensemble of  $N$  qubits labeled with  $i$  and  $j$  index. Those qubits interacts with an ising-type interaction (pair wise spin interaction)

$$\hat{H}_{int} = - \sum_{i,j} J_{ij} \hat{Z}_i \hat{Z}_j,$$

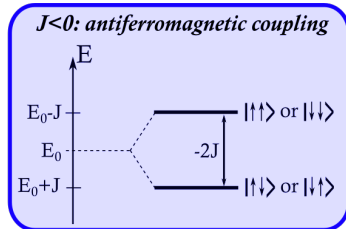
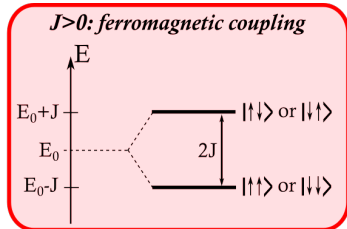
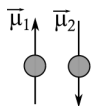
where  $J_{ij}$  is the intensity of interaction between qubits  $i$  and  $j$ .

# 1.1. Ising interaction

It corresponds to a generic two-qubits interaction

$$\hat{H}_{int} = -J\hat{Z}_1\hat{Z}_2,$$

with  $J > 0$  for a ferromagnetic coupling, and  $J < 0$  for an anti-ferromagnetic coupling.



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## 1.2. Two-qubit unitary evolution

Applying the hamiltonian

$$\hat{H}_{int} = -J\hat{Z}_1\hat{Z}_2,$$

for a time  $T$ , the unitary evolution will be

$$\hat{C}(\gamma) = e^{-i\frac{\gamma}{2}\hat{Z}_1\hat{Z}_2},$$

with

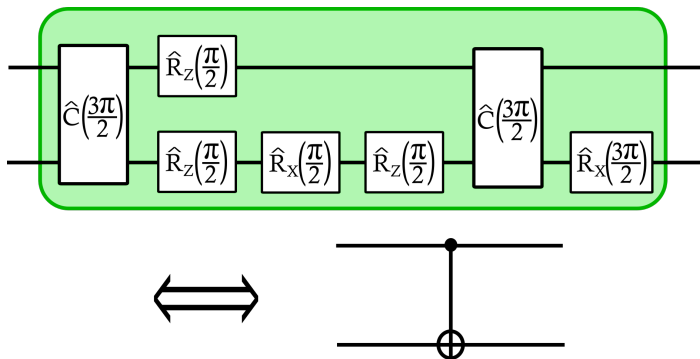
$$\gamma = -\frac{2J}{\hbar}T.$$

$\hat{C}(\gamma)$  **does not realize a C-NOT gate yet.** Additionally, single qubit operations on each of the qubits are required to realize a C-NOT gate as follow

$$e^{-i\frac{3\pi}{4}}\hat{R}_{X2}\left(\frac{3\pi}{2}\right)\hat{C}\left(\frac{3\pi}{2}\right)\hat{R}_{Z2}\left(\frac{\pi}{2}\right)\hat{R}_{X2}\left(\frac{\pi}{2}\right)\hat{R}_{Z2}\left(\frac{\pi}{2}\right)\hat{R}_{Z1}\left(\frac{\pi}{2}\right)\hat{C}\left(\frac{3\pi}{2}\right)$$

## 1.2. Two-qubit unitary evolution

Circuit representation of a C-NOT gate made with a two-qubit interaction  $\hat{C}(\gamma)$



Any physical two-qubit interaction that can produce entanglement can be tuned into a universal two-qubit gate (such as the C-NOT gate) when it is augmented by arbitrary single qubit operations.

Ref: Bremner *et al.*, Physical Review Letter, **89**, 247902 (2002).

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## II.1. NMR quantum computing

NMR is based on manipulation and measurement of nuclear spins. It's well adapted for quantum computing implementation and the first quantum calculation was implemented in NMR systems.

Reference:

Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance, Nature, **414**, 883-887 (2001).

⇒ factorization of  $15 = 3 \times 5$  in molecules by NMR.

### Introduction review articles

- NMR techniques for quantum control and computation, Rev. Mod. Phys., **76** (2004)
- Bulk spin-resonance quantum computation, Science, **275**, 350 (1997)

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## II.2. Manipulation of qubits and NMR

- **Qubits:** nuclear spins  $1/2$  in  $\vec{B}_0$  ( $|\uparrow\rangle$  and  $|\downarrow\rangle$  as  $|0\rangle$  and  $|1\rangle$ ).
- **Quantum gates:** RF pulses and delay times.
- **Input:** Boltzmann distribution of spins (room temperature).
- **Read out:** detect spin states with RF coil.
- **Coherence times:** easily several seconds.



## II.2. Manipulation of qubits and NMR

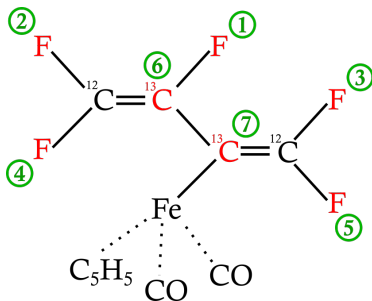
Nuclear spin in a static  $\vec{B}_0$  field, with  $\hat{I}$  the nuclear spin operator and  $\vec{B}_0 = B_0 \vec{u}_z$ ,

$$\hat{\mathcal{H}}_0 = -\hbar\gamma B_0 \hat{I}_Z = -\frac{\hbar\omega_0}{2} \hat{Z},$$

where  $\omega_0$  is the Larmor frequency: precession of the qubit around  $\vec{u}_z$  at Larmor frequency.

## II.2. Manipulation of qubits and NMR

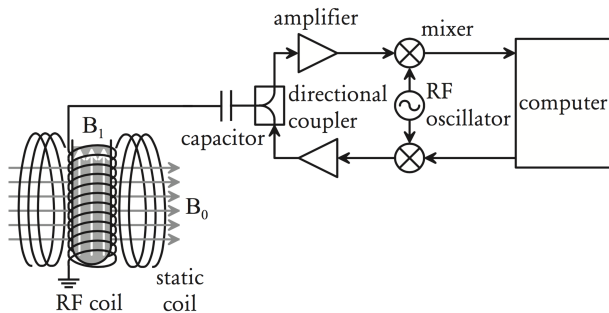
Case of  $C_4F_5Fe(CH)_5(CO)_2$  - perfluorobutadienyl iron complex.  
Vendersypen *et al.*, Nature **414**, 883 (2001).



Nuclei labeled in red are qubits (F and <sup>13</sup>C), numbered in green.

$$B_0 = 11,7T.$$

## II.2. Manipulation of qubits and NMR



I. L. Chuang et al., Proceedings of the Royal Society A 454, pp. 447-467 (1998).

## II.2. Manipulation of qubits and NMR

Even without qubit/qubit coupling, the Larmor frequency depends on the atoms. Those frequencies are shifted depending on the coupling with the chemical environment

$$\mathcal{H}_0 = - \sum_{j=1}^n \hbar(1 - \tilde{\sigma}_j)\gamma_j B_0 \hat{I}_Z^j = - \sum_{i=1}^n \frac{\hbar}{2} \omega_0^i (1 - \tilde{\sigma}_i),$$

with  $\omega_0^i$  the Larmor frequency of the nuclei  $i$  without qubit/qubit coupling and  $\tilde{\sigma}_i$  the chemical frequency shift due to coupling with neighboring spins.

$\tilde{\sigma}_i$  is used in analytical chemistry to determine the environment of an atom, while here it is used to address different qubits with different RF frequencies independently.

## II.2. Manipulation of qubits and NMR

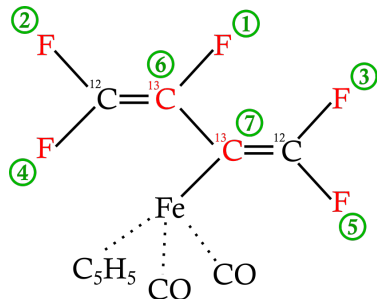
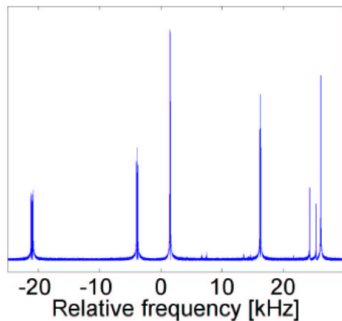
**Exemple:** Larmor frequency at 11.7 T for different atoms

| Atom            | $\omega_0^i$ |
|-----------------|--------------|
| $^1\text{H}$    | 500 MHz      |
| $^{13}\text{C}$ | 126 MHz      |
| $^{15}\text{N}$ | -51 MHz      |
| $^{19}\text{F}$ | 470 MHz      |
| $^{31}\text{P}$ | 202 MHz      |

with 500 MHz equivalent to 25 mK.

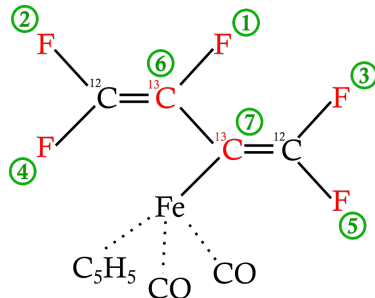
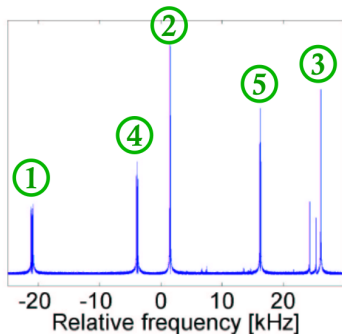
## II.2. Manipulation of qubits and NMR

Chemical shifts of the five F qubits of perfluorobutadienyl iron complex



## II.2. Manipulation of qubits and NMR

Chemical shifts of the five F qubits of perfluorobutadienyl iron complex



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## 11.3. RF field interaction: single qubit rotation

In the rotating frame and the rotating wave approximation, the hamiltonian becomes

$$\hat{H}^{rot} = -\frac{\hbar\delta}{2}\hat{Z} - \frac{\hbar\omega_1}{2}\left(\cos\phi\hat{X} + \sin\phi\hat{Y}\right),$$

with  $\delta = \omega_0 - \omega_{RF}$  the detuning between RF and Larmor frequency,  $\phi$  the phase of the RF field and  $\omega_1 = \gamma B_1$  where  $B_1$  is the amplitude of the RF field.

For  $n$  qubits of Larmor frequencies  $\omega_0^i$ , gyromagnetic factor  $\gamma_i$  and  $\omega_1^i = \gamma_i B_1$ , frequency shift  $\tilde{\sigma}_i$ , one notes

$$\delta_i = \omega_0^i (1 - \tilde{\sigma}_i) - \omega_{RF},$$

the detuning between RF and qubit  $i$  frequency, such that

$$\hat{H}^{rot} = -\sum_{i=1}^n \frac{\hbar}{2} \delta_i \hat{Z}_i - \frac{\hbar}{2} \sum_{i=1}^n \left( \cos \phi \omega_1^i \hat{X}_i + \sin \phi \omega_1^i \hat{Y}_i \right).$$

## II.3. RF field interaction: single qubit rotation

Let call  $T$  the time during which the RF field is applied to the system of  $n$  qubits. If  $T$  is long enough, each spin resonance is non overlapping with the others. So if  $\omega_{RF}$  is not close enough to a Larmor frequency corrected  $\omega_0^i (1 - \tilde{\sigma}_i)$ , the effect of the RF field is negligible. If  $\omega_{RF} \approx \omega_0^i (1 - \tilde{\sigma}_i)$ , only the qubit  $i$  will be affected and rotate on the Bloch sphere.

**If qubits have different Larmor frequencies, it is possible to manipulate each qubit individually choosing the corresponding frequency.**

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## 11.4. Coupled spins

When spins of different atoms are coupled, the coupling interaction energy usually results in level splitting. Consequently, the Larmor frequency of a qubit, corrected by the chemical frequency shift  $\tilde{\sigma}_i$ , will depend on the state of neighborhooding qubits.

In other words, the resonance RF frequency of a qubit will depend on the state of the neighborhooding qubits.

**This phenomena is the key physical effect used to implement multiqubit gates.**

## 11.4. Coupled spins

The coupling hamiltonian might be written as follow

$$\hat{H}_J = \hbar \sum_{i < j} 4J_{ij} \hat{I}_Z^i \hat{I}_Z^j,$$

$$\hat{H}_J = \hbar \sum_{i < j} J_{ij} \hat{Z}^i \hat{Z}^j.$$

$J > 0$ : antiferromagnetic interaction,

$J < 0$ : ferromagnetic interaction.

## II.4. Coupled spins

Coupling constants of the five F qubits of perfluorobutadienyl iron complex

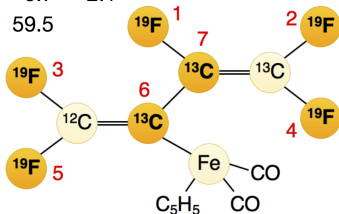
| $i$ | $\omega_i/2\pi$ | $T_{1,i}$ | $T_{2,i}$ | $J_{7i}$ | $J_{6i}$ | $J_{5i}$ | $J_{4i}$ | $J_{3i}$ | $J_{2i}$ |
|-----|-----------------|-----------|-----------|----------|----------|----------|----------|----------|----------|
| 1   | -22052.0        | 5.0       | 1.3       | -221.0   | 37.7     | 6.6      | -114.3   | 14.5     | 25.16    |
| 2   | 489.5           | 13.7      | 1.8       | 18.6     | -3.9     | 2.5      | 79.9     | 3.9      |          |
| 3   | 25088.3         | 3.0       | 2.5       | 1.0      | -13.5    | 41.6     | 12.9     |          |          |
| 4   | -4918.7         | 10.0      | 1.7       | 54.1     | -5.7     | 2.1      |          |          |          |
| 5   | 15186.6         | 2.8       | 1.8       | 19.4     | 59.5     |          |          |          |          |
| 6   | -4519.1         | 45.4      | 2.0       | 68.9     |          |          |          |          |          |
| 7   | 4244.3          | 31.6      | 2.0       |          |          |          |          |          |          |

At  $B_0 = 11.7$  T:

$\omega_{0,F}/2\pi = 470$  MHz

$\omega_{0,C}/2\pi = 125$  MHz

$[\omega_i/2\pi] = \text{Hz}$ ,  $[T] = \text{s}$ ,  $[J] = \text{Hz}$



L. M. K. Vandersypen et al., Nature 414, 883 (2001)

5 resonances frequencies corresponding to 5 different qubits.

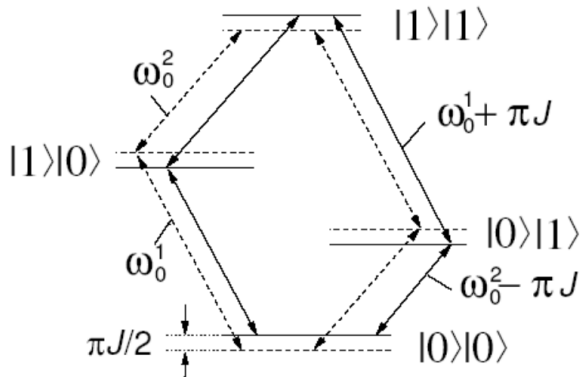
## II.4. Coupled spins

**Orders of magnitude:** in the case of perfluorobutadienyl iron complex at 11,7T

- Larmor frequency of F-type qubit  $\sim 470$  MHz ;
- chemical frequency shift  $\sim 10 - 20$  kHz;
- typical RF strength  $\omega_1 \sim 2\pi \times 100$  kHz ;
- typical level splitting due to qubit/qubit coupling  $J \sim \text{few } 100$  Hz max.

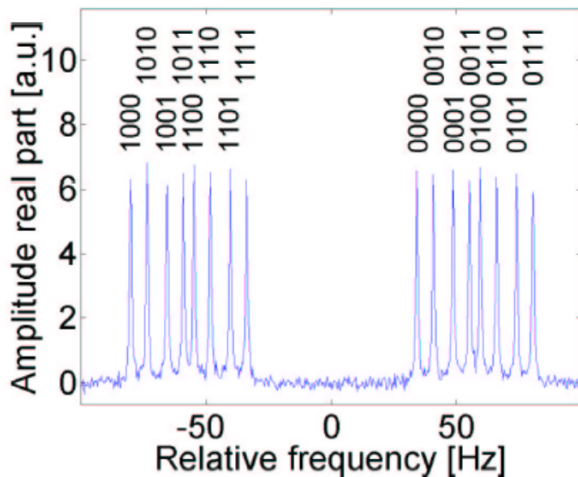
$$\frac{100 \text{ Hz}}{470 \text{ MHz}} \sim 2 \cdot 10^{-7}, \quad \frac{100 \text{ Hz}}{10 \text{ kHz}} \sim 10^{-2}.$$

## 11.4. Coupled spins





## II.4. Coupled spins



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## 11.5. Controlled-NOT gate in NMR

Two spins  $A$  and  $B$  as qubits. C-NOT gate flips  $A$  if  $B$  is  $\downarrow$ .

| Before       |              | After        |              |
|--------------|--------------|--------------|--------------|
| $A$          | $B$          | $A$          | $B$          |
| $\uparrow$   | $\uparrow$   | $\uparrow$   | $\uparrow$   |
| $\uparrow$   | $\downarrow$ | $\downarrow$ | $\downarrow$ |
| $\downarrow$ | $\uparrow$   | $\downarrow$ | $\uparrow$   |
| $\downarrow$ | $\downarrow$ | $\uparrow$   | $\downarrow$ |

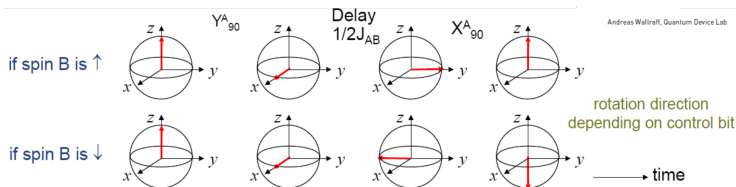
## 11.5. Controlled-NOT gate in NMR

**Sequence:**

Apply  $\hat{R}_{Y,A}(\frac{\pi}{2})$ , wait for a delay

$$\Delta t = \frac{\pi}{4J_{AB}},$$

and finally apply  $\hat{R}_{X,A}(\frac{\pi}{2})$ . Let describe this sequence on the Bloch sphere of spin A in the rotating frame at the larmor frequency of A,  $\nu_A$  (no coupling).

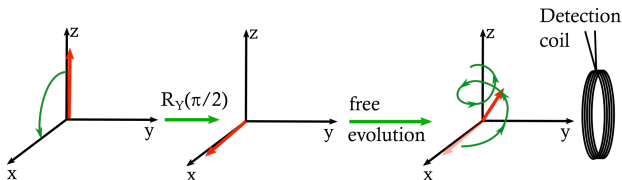


The rotation direction depends on the control qubit.

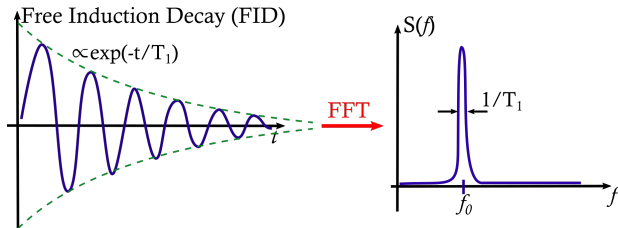
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## II.6. Read-out in NMR

Based on NMR method. Apply  $\hat{R}_Y(\frac{\pi}{2})$  pulse and measure spin relaxation signal

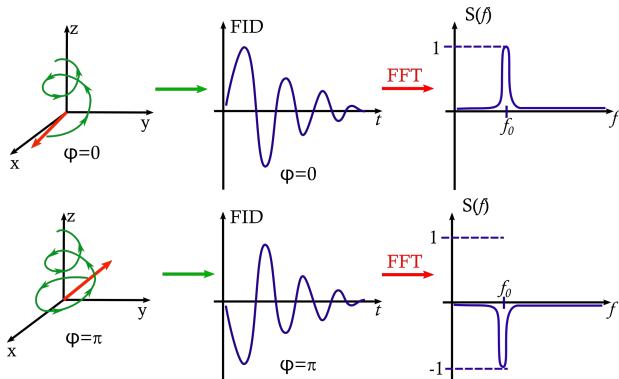


A coil measures the free evolution of the spin to get access to the so-called free induction decay signal and afterwards the integrated signal or the spectrum by FFT



## II.6. Read-out in NMR

Depending on the initial position of the equator of the Bloch sphere, the phase of the free induction decay will be different

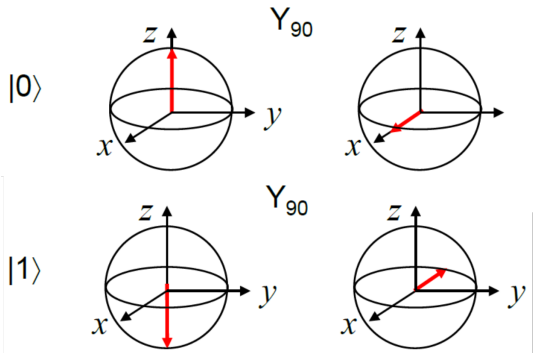


The initial angle  $\varphi$  on the Bloch sphere is measured by the FID signal in NMR.

## 11.6. Read-out in NMR

NMR is a phase sensitive detection method. A qubit state is measured with a as follow

Andreas Wallraff, Quantum Device Lab



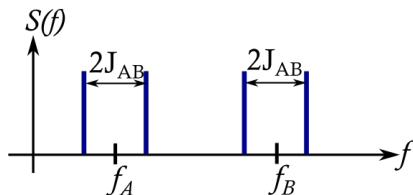
For a  $|0\rangle$  state,  $\varphi = 0$  after the  $\hat{R}_Y(\frac{\pi}{2})$  pulse leading in a positive signal in the FFT of FID.

For a  $|1\rangle$  state,  $\varphi = \pi$  after the  $\hat{R}_Y(\frac{\pi}{2})$  pulse leading in a negative signal in the FFT of FID.



## 11.6. Read-out in NMR

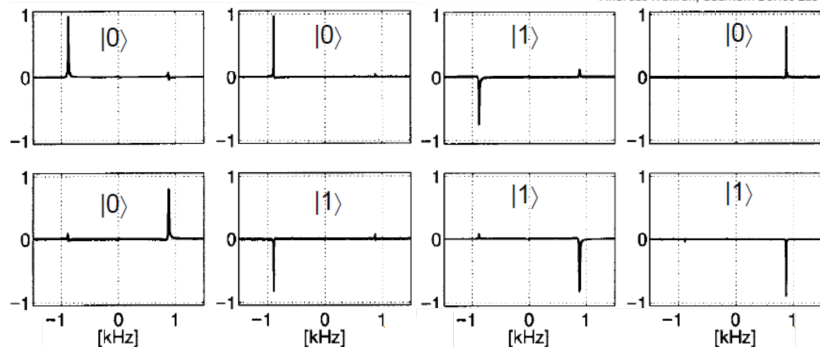
Two coupled qubits in their four computational basis states have the following spectrum



NMR detection signal (FFT of FID) depends on states.

## II.6. Read-out in NMR

Andreas Wallraff, Quantum Device Lab



It's easier and faster experimentally to detect the sign of  $S(\nu)$  rather than the frequency shift  $J_{AB}$  which is only of few hundreds of Hz.

**State detection is based on sign measurement of the NMR signal  $S(\nu)$ .**

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## 11.7. Example of Shor's algorithm

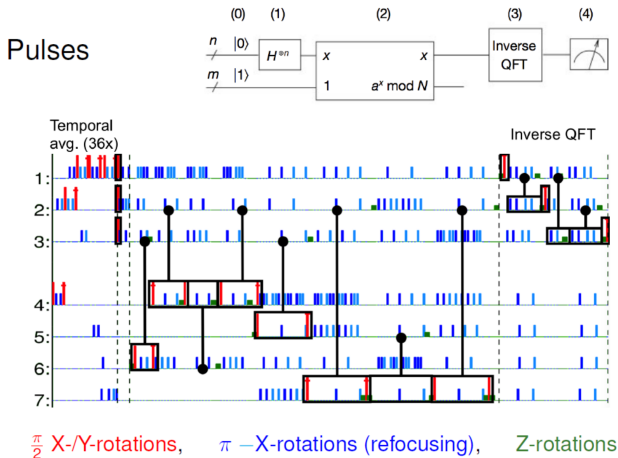
Real sequence in practice for factorization with perfluorobutadienyl iron complex.

Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance, Nature, **414**, 883-887 (2001).

⇒ factorization of  $15 = 3 \times 5$  in molecules by NMR with Shor's algorithm.

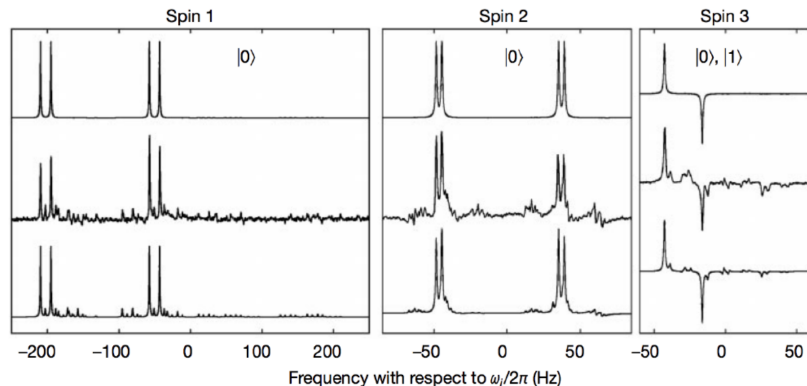
## 11.7. Example of Shor's algorithm

Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance, *Nature*, **414**, 883-887 (2001).



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## 11.8. Quantum state tomography

It is possible to reconstruct a state after a quantum calculation if it's not a pure state  $|0\rangle$  or  $|1\rangle$ .

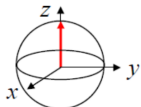
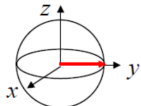
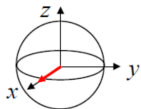
It is however possible to reconstruct a quantum state if it is possible to produce it several times. The principle consists in applying different rotations to look at the qubits from different angle.

It is called **quantum state tomography**.

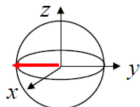
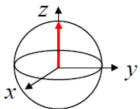
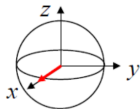


# II.8. Quantum state tomography

initial state  
no pulse

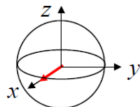
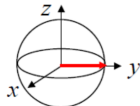
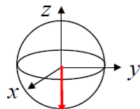


after  $X_{90}$



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after  $Y_{90}$



- 1 Implementation of a C-NOT gate
- 2 Example with NMR quantum computing
- 3 Molecules for quantum computing based on NMR techniques
  - Properties of molecules
  - Examples of molecules used

# Implementation of multiqubit gates - Case of NMR

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## III.1. NMR quantum computing

A quantum computer is a known molecule with the following desired properties

- spins  $1/2$  ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{15}\text{N}$ ,...) ;
- long  $T_1$ 's and  $T_2$ 's ;
- heteronuclear, or large chemical shifts (required to address different spin types independently) ;
- good  $J$ -coupling network (clock-speed) ;
- stable, available, soluble,...

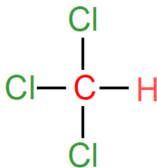
# Implementation of multiqubit gates - Case of NMR

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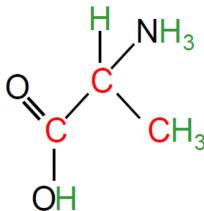
## III.2. Examples of molecules used

red nuclei are used  
as qubits:

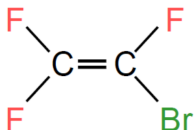
Grover / Deutsch-Jozsa



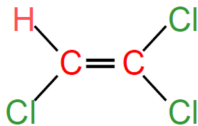
Q. Error correction



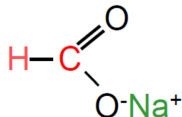
Logical labeling / Grover



Teleportation



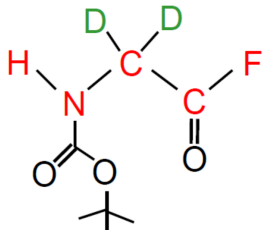
Q. Error Detection



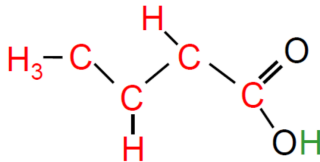
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## III.2. Examples of molecules used

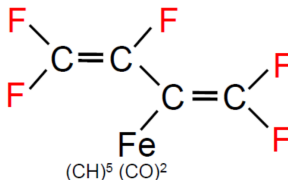
Deutsch-Jozsa



7-spin coherence

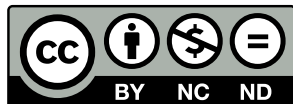


Order-finding



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