

# NMR Quantum Information Processing

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# Goal of the lectures

**Give a sketch how to use spin degrees of freedom for quantum information processing.** We'll do that by giving an introduction to NMR quantum information processing, from basic ideas to some of the most recent developments with a focus on the control of multiqubit systems (up to a dozen qubits). Then we will turn to solid state NMR, and discuss some recent directions. We will give an assessment of the important achievements and point toward future developments.

# Other groups

## NMR QIP around the world

- David Cory's group at MIT
- Yoshi Yamamoto in Stanford
- Michael Meihring in Stuttgart
- Sefan Glazer in Munich
- Jonathan Jones at Oxford
- Ike Chuang at MIT
- Dieter Sutter in Dortmund
- ...

# Plan

- 1. Nuclear Magnetic Resonance (NMR) QIP
  - Qubits and Gates
  - Measurement
  - Initial states
  - Noise
  - Isolate the spin  $3/2$
- 2. Some benchmarks/algorithms implemented
  - Quantum error correction:  
3/5 bit codes, noiseless subsystems
  - Physics simulation
  - The power of one bit of quantum information

# Plan

- **3. Solid state NMR**

- **Similarities and difference between liquid and solid**
- **Control of solid state NMR qubits**
- **Heat bath algorithmic cooling**

# Main reference

“Introduction to NMR Quantum Information Processing” [2],  
R. Laflamme,  
E. Knill, D. G. Cory, E. M. Fortunato,  
T. Havel, C. Miquel, R. Martinez,  
C. Negrevergne, G. Ortiz,  
M. A. Pravia, Y. Sharf, S. Sinha,  
R. Somma and L. Viola,  
Los Alamos Science  
Number 27 p. 226-259, or  
[quant-ph/0207172](https://arxiv.org/abs/quant-ph/0207172).



This can also be found at  
[www.iqc.ca/publications/tutorials/inmrqip.pdf](http://www.iqc.ca/publications/tutorials/inmrqip.pdf)

# Notation

- Pauli matrices:

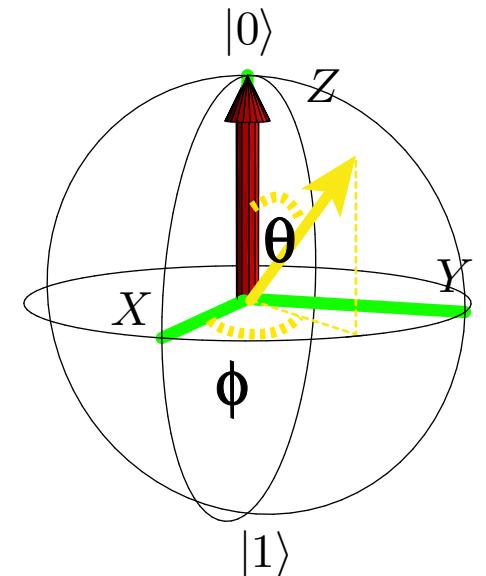
$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = Y = \begin{pmatrix} 0 & -i \\ 0 & i \end{pmatrix}; \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Tensor product  $X_k = \mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes X \otimes \cdots \otimes \mathbb{1}$ .

- Bloch sphere: a geometric representation of the state

$$\Psi = \cos \theta |0\rangle + e^{i\phi} \sin \theta |1\rangle \text{ or}$$

$$\rho = \frac{1}{2}(\mathbb{1} + \sin[\theta] \cos[\phi]X + \sin[\theta] \sin[\phi]Y + \cos[\theta]Z)$$



- $\hbar = 1.05 \times 10^{-34} \text{ Js}$ ,  $k = 1.38 \times 10^{-23} \text{ J/K}$

1 Tesla =  $10^4$  Gauss (Earth Magnetic field = 0.5 Gauss)

$\mu_p = 26.75 \times 10^7 / (\text{Ts})$

- Freq. of the spectrometer  $\nu_L^p = 26.75 \times 10^7 \text{ rad/(Ts)} * 11.7T/2\pi = 500 \text{ MHz}$

- Corresponding  $\beta = \hbar \times \omega_l / kT$

$$= 1.05 \times 10^{-34} \text{ Js} \times 2\pi \times 486 \text{ MHz} / (1.38 \times 10^{-23} \text{ J/K} \times 300 \text{ K}) \approx 7.8 \times 10^{-5}$$

- Definition of  $T_1$  (relaxation time):  $M_z(\tau) = M_z^0[1 - 2e^{(-\tau/T_1)}]$

- Definition of  $T_2$  (decoherence time):  $M_x(\tau) = M_x^0[\exp(-2\tau/T_2)]$

# Liquid state NMR QIP

Thanks to

IQC NMR group: C. Negrevergne, C. Ryan, J. Boileau, M. Laforest,  
F.Y. Cyr-Racine, B. Power, M. Ditty

Perimeter Institute: H. Ollivier



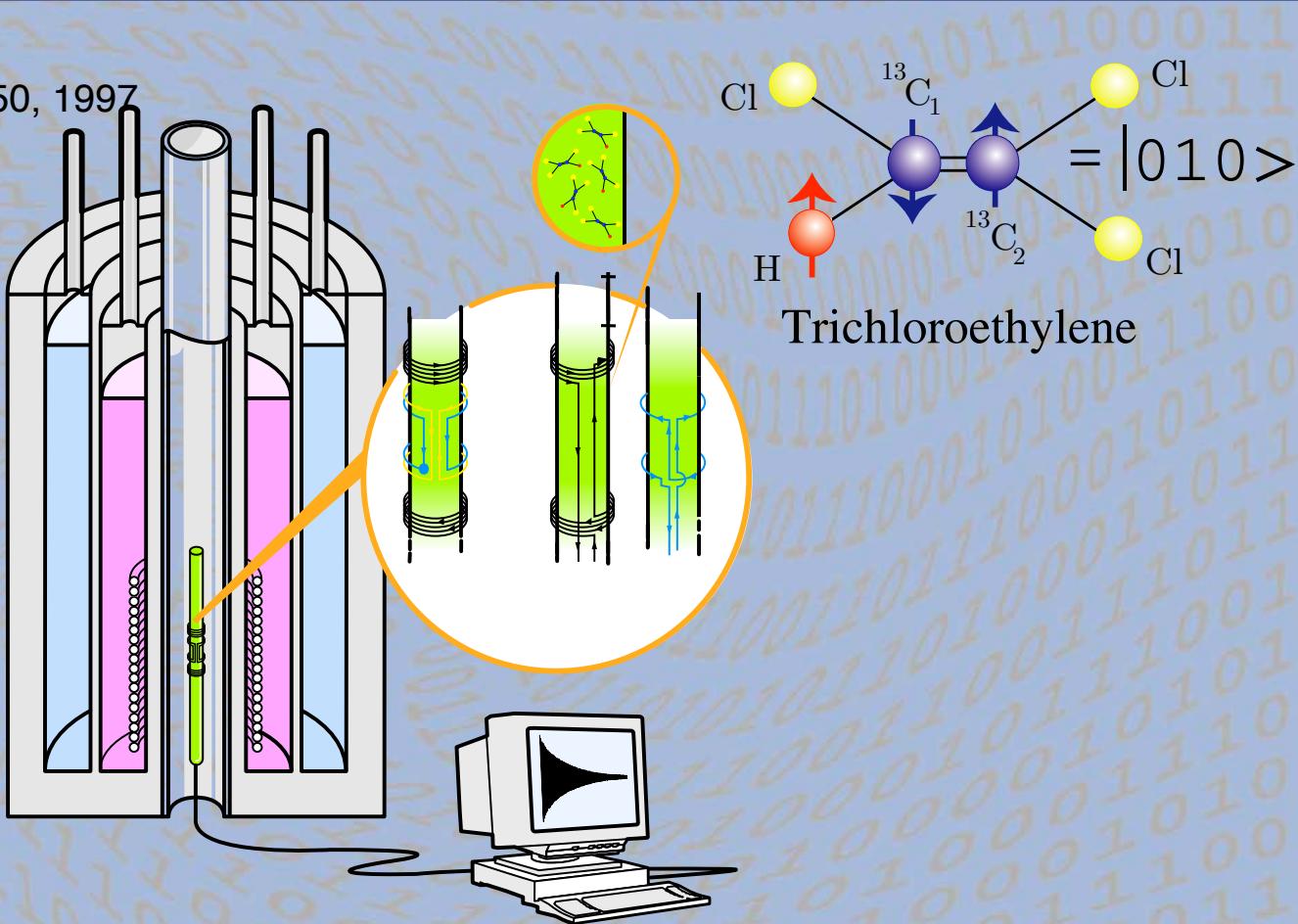
MIT group: C. Ramanathan, S. Sinha, H-J Cho, T. Havel, D. Cory

# NMR QIP overview

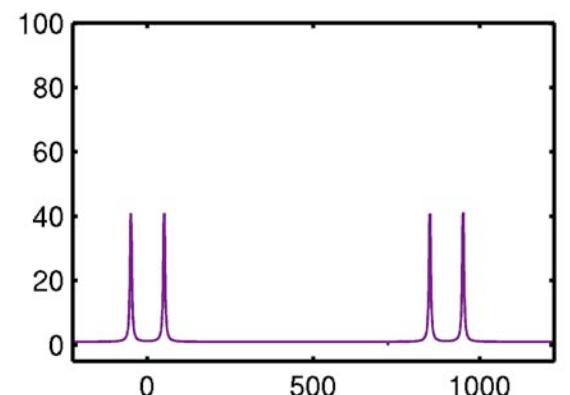
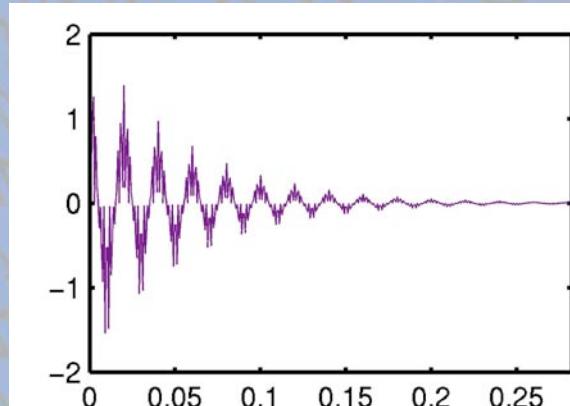
Cory & Havel PNAS, 64, 1634, 1997

Gershenfeld & Chuang, Science 275, 350, 1997

- Larmor frequency  $\sim 500$  MHz
- Single bit gate:  $\sim 1/\text{kHz} \sim \text{ms}$   
 $H_{sb} \sim \omega_l \sigma_z^1$
- Two bit gate  $\sim 10$  ms:  $\sigma_z^1 \sigma_z^2$   
 $H_{int} \sim J \sigma_z^1 \sigma_z^2$
- $T_2 \sim 1\text{s}$



Bruker DRX-500



# The qubits

- Some atoms, like hydrogen, carbon 13, have nuclei which possess a magnetic moment  $\vec{\mu} = \mu \vec{I}$  where  $\vec{I}$  is the angular momentum operator for a spin half system.

The Hamiltonian is given by

$$H = \vec{\mu} \cdot \vec{B}$$

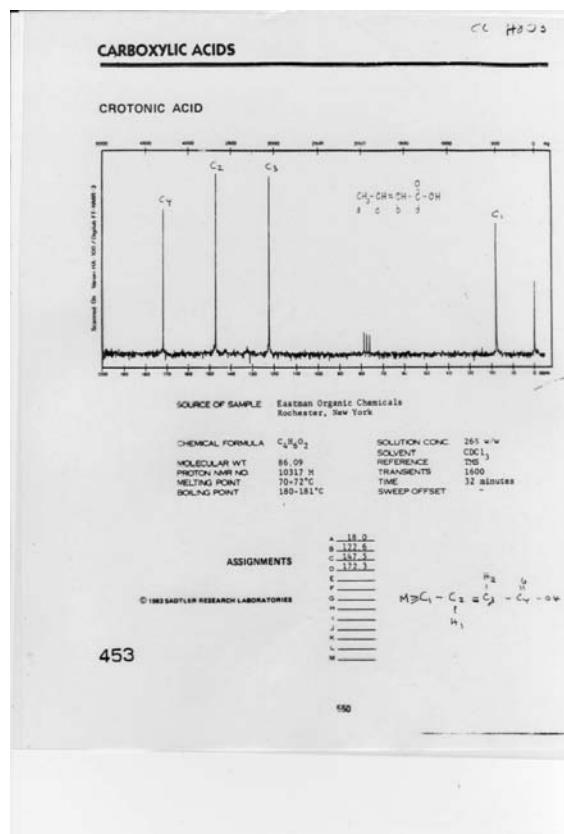
where  $\vec{B}$  is the magnetic field.

- Use  $B_o \hat{z}$ , this implies  $H = \mu B_o Z$ . This field will induce a rotation of the magnetic moment around the  $z$  axis at frequency called the Larmor frequency  $\omega^L = \mu B_o$ .

- Although all nuclei of the same species have the same magnetic moment, the surrounding electrons in a molecule are able to shield to various degree the external magnetic field. This leads to an effective magnetic moment. The difference between the value of an isolated nucleus and the one observed is called the chemical shift and is denoted by  $\delta$ . The chemical shift is how the different qubits are distinguished. (This is not necessary, ideas from cellular automata can be used ... but we won't here).
- We will often go in the rotating frame of each nuclei, one which rotates at each of the Larmor frequency of the nuclei implemented by the transformation:  $e^{-i(\omega_1^L Z_1 + \omega_2^L Z_2 + \dots)t}$ . This “easy” to track, and is computationally efficient. The evolution in this multi-rotated frame will look simpler.

# The choice of molecule

- Large chemical shift
- Large J coupling
- Large decoherence time



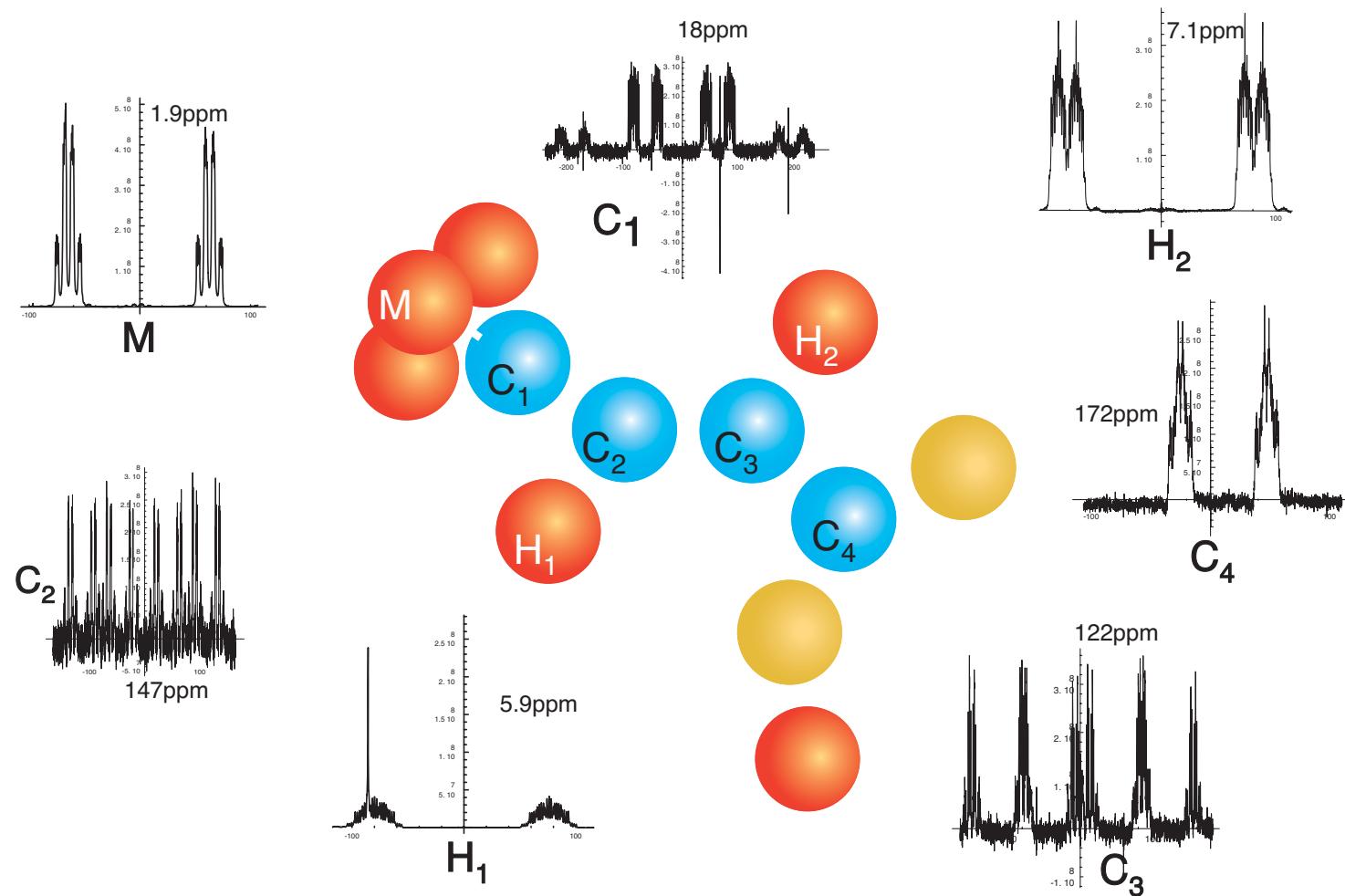
Rudy Martinez, Stable Isotope Lab, Los Alamos

	M	H <sub>1</sub>	H <sub>2</sub>	C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>
M	-969.4						
H <sub>1</sub>	6.9	-3560.3					
H <sub>2</sub>	-1.7	15.5	-2938.2				
C <sub>1</sub>	127.5	3.8	6.2	-2327.0			
C <sub>2</sub>	-7.1	156.0	-0.7	41.6	-18599.2		
C <sub>3</sub>	6.6	-1.8	162.9	1.6	69.7	-15412.8	
C <sub>4</sub>	-0.9	6.5	3.3	7.1	1.4	72.4	-21685.1

Chemical structure diagram showing the positions of the carbons and hydrogens relative to the methyl group (M) and the carboxylic acid group (-COOH). The methyl group is labeled M. The methylene group is labeled C<sub>1</sub>. The two hydrogens on the methylene group are labeled H<sub>1</sub> and H<sub>2</sub>. The carbonyl carbon is labeled C<sub>2</sub>. The two hydrogens on the carbonyl carbon are labeled H<sub>3</sub> and H<sub>4</sub>. The carbon-carbon double bond is labeled C<sub>3</sub>. The two hydrogens on the carbon-carbon double bond are labeled H<sub>5</sub> and H<sub>6</sub>. The carbon atom of the carboxylic acid group is labeled C<sub>4</sub>.

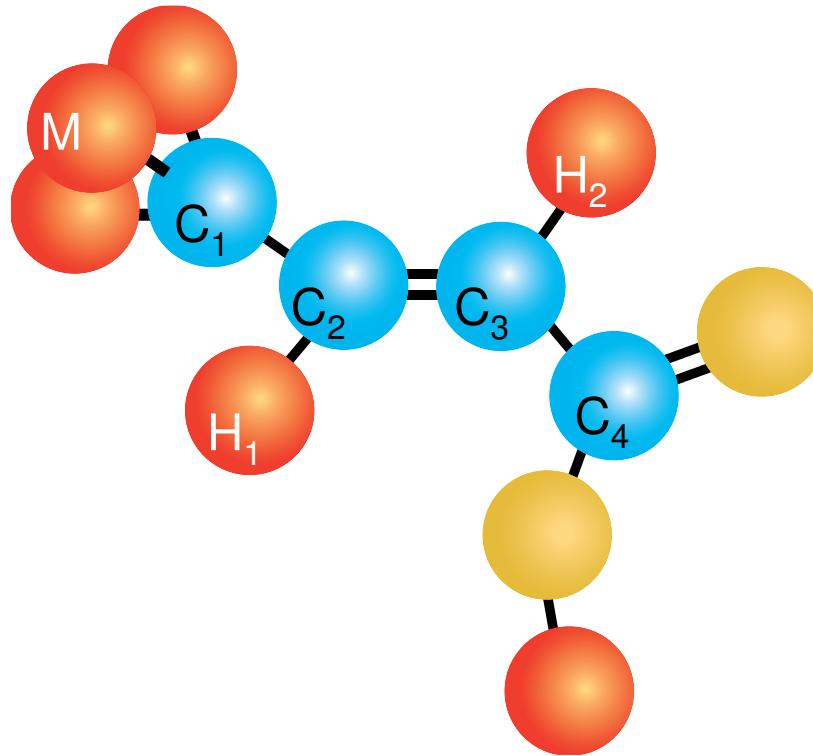
# Spectra of crotonic acid

## Crotonic acid



# Hilbert space

Breaking a Hilbert space into qubits:



- Breaking the methyl hydrogens into spin 3/2 and spin 1/2 components (in fact there are two spin 1/2, and they can be decomposed into a symmetric and non-symmetric part, our control is on the symmetric part only).

# Control: one bit gate

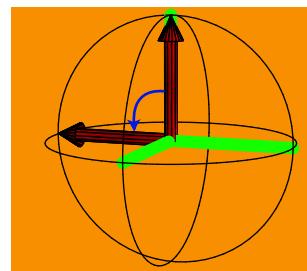
$$H = \sum_i \vec{\mu}_i \cdot \vec{B} = H_b + H_{rf}$$

- The background field  $\vec{B}_b = B_b \hat{z}$  :  $H_b = \sum_i \omega_L^i Z_i$ .
- To induce one bit gates use the coil to send rf waves  $\vec{B}_{rf} = B_x \cos[\omega_L(t - t_0)] \hat{x} + B_y \sin[\omega_L(t - t_0)] \hat{y}$  which looks like a constant magnetic field in the rotating frame.

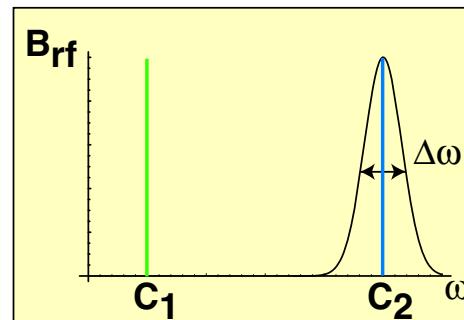
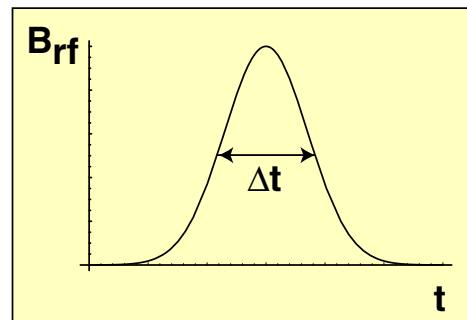
Rotation around x/y axis: e.g. around x

Rotation around z axis:

hard pulse: 10  $\mu\text{s}$ ;  
soft pulse  $1/\delta$



$$\begin{aligned}e^{-i\theta X} &= \mathbb{1} \cos[\theta] - iX \sin[\theta] \\Z &\rightarrow Z \cos[2\theta] - Y \sin[2\theta] \\Y &\rightarrow Y \cos[2\theta] + Z \sin[2\theta]\end{aligned}$$



# A universal set of one bit gates

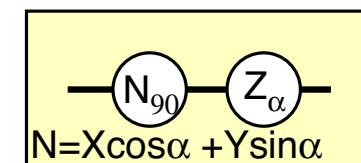
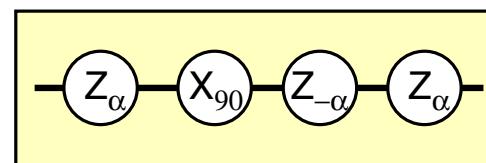
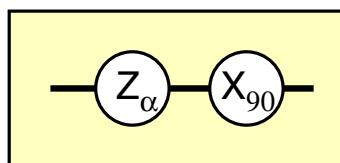
In NMR, the background Hamiltonian provides rotation around the z axis, and only rotation of 90° around the x-axis are necessary to obtain universality.

A generic rotation can be written as:  $e^{-i\theta\vec{n}\cdot\vec{\sigma}}$  which can be rewritten as

$$e^{-i\frac{\alpha}{2}Z} e^{i\frac{\pi}{4}X} e^{i\frac{\beta}{2}Z} e^{-i\frac{\pi}{4}X} e^{-i\frac{\theta}{2}Z} e^{i\frac{\pi}{4}X} e^{-i\frac{\beta}{2}Z} e^{-i\frac{\pi}{4}X} e^{-i\frac{\alpha}{2}Z}$$

$$\alpha = \tan^{-1}[n_y/n_x] : \beta = \tan^{-1}[n_x/n_z]$$

In NMR, we have rotation around axis on the X – Y plane and Z rotations come for free as they can be done by redefining subsequent rotation axis of rotation:



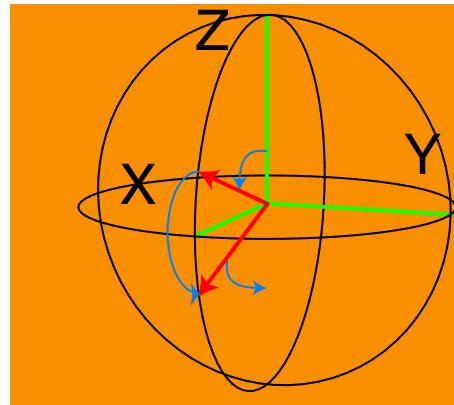
we usually limit ourselves to 90° or 180° as they are easier to calibrate.

# Pulse with increased robustness

Suppose we are not able to calibrate very well and a  $90^\circ$  is really  $90^\circ + \epsilon$ , how can we make a pulse which reduce this imprecision?

For  $Z$  initial state, use the sequence:

$$U = e^{-i(\frac{\pi}{4}+\epsilon)Y} e^{-i(\frac{\pi}{2}+2\epsilon)X} e^{-i(\frac{\pi}{4}+\epsilon)Y}$$



For a general state we need the sequence

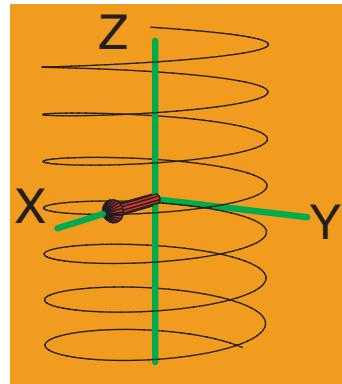
$$U = e^{-i\frac{\pi}{2}X} e^{-i\frac{\pi}{2}(X \cos[-30] + Y \sin[-30])} e^{-i\frac{\pi}{2}(X \cos[60] + Y \sin[60])} \\ e^{-i\frac{\pi}{2}(X \cos[-30] + Y \sin[-30])} e^{-i\frac{\pi}{2}X}$$

Exercise: Show that if  $\frac{\pi}{2} \rightarrow \frac{\pi}{2} + \epsilon$ , the gate remains precise to order  $\epsilon^2$ .

# Control: gradient fields

Remember  $H_{grad} = \vec{\mu} \cdot \vec{B}_{grad}$  and use a gradient field  $\vec{B}_{grad} = B_{grad} z \hat{z}$

The sample get a linear phase as a function  $z$ :



$$I_{\pm}(z) = X \pm iY \rightarrow e^{-(\pm)i\mu B_{grad} z t} I_{\pm}$$

The operators  $I_{\pm}$  gets averaged over  $z$ .

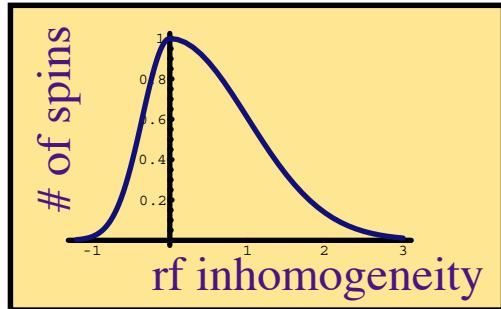
- We can use this to “label” parts of the density matrix, e.g. the one with different number of  $I_{\pm}$ .

$$\begin{aligned} I_+^1 \mathbb{1} &\rightarrow e^{-i\mu B_{grad} z} I_+ \quad ; \quad I_+^1 I_+^2 \rightarrow e^{-i2\mu B_{grad} z} I_+^1 I_+^2 \\ I_+^1 I_-^2 &\rightarrow I_+^1 I_-^2 \quad ; \quad Z^1 \mathbb{1} \rightarrow Z^1 \mathbb{1} \end{aligned}$$

$$\langle I_{\pm} \rangle_z = \int_{-z_l/2}^{z_l/2} dz e^{-i\mu B_{grad} z} I_{\pm} \sim \frac{1}{\mu B_{grad} z_l}$$

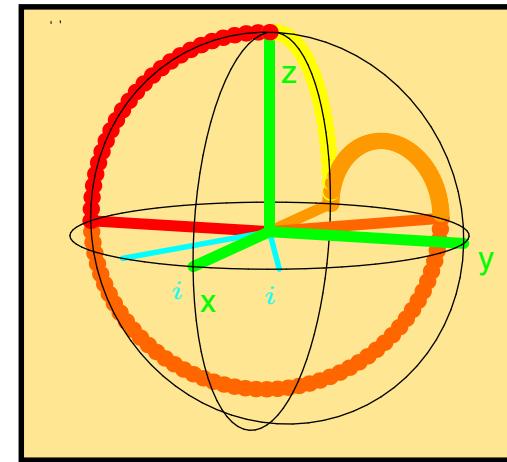
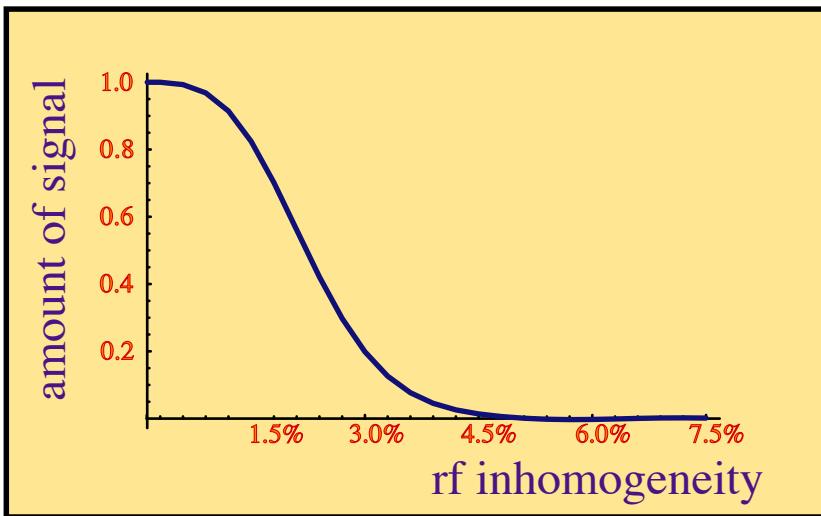
- Gradients can also be used to implement decoherence.

# Control: rf selection



The rf power is different for various parts of the sample: we need to find a way to either homogenize or use a sub-sample of the spin where this inhomogeneity is reduced

$$R_x^{90} (R_{-X}^{180})^{64} (R_{\phi_i}^{180} R_{-\phi_i}^{180})^{64} R_Y^{90} + \text{Gradient}$$
$$\sum_i \phi_i = \pi/8$$



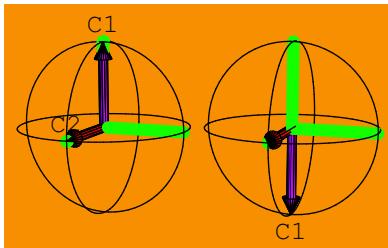
Get homogeneity up to +/- 2%  
(with around 12% of the signal)

# Control: two bit gates

- Indirect interaction between spins (mediated through electrons)

$$H_{int} = \sum_{ij} J_{ij} \vec{\sigma}^i \cdot \vec{\sigma}^j = \sum_{ij} J_{ij} (X^i X^j + Y^i Y^j + Z^i Z^j)$$

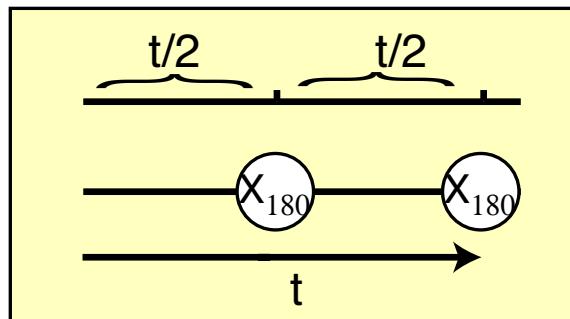
If  $|\omega_L^i - \omega_L^j| \ll J_{ij}$ , we can neglect  $X^i X^j + Y^i Y^j$



$$\begin{aligned} e^{-i\phi ZZ} &= \mathbb{1}\mathbb{1} \cos \phi - iZZ \sin \phi \\ X\mathbb{1} &\rightarrow X\mathbb{1} \cos 2\phi + YZ \sin 2\phi \\ Y\mathbb{1} &\rightarrow Y\mathbb{1} \cos 2\phi - XZ \sin 2\phi \end{aligned}$$

- Eliminate the natural evolution using refocusing

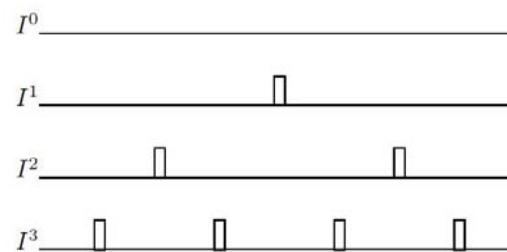
$$\mathbb{1} = \underbrace{e^{i\pi X/2} e^{-i\pi J_{12}t Z^1 Z^2/2} e^{-i\pi X/2}}_{e^{i\pi J_{12}t Z^1 Z^2/2}} e^{-i\pi J_{12}t Z^1 Z^2/2}$$



Can we refocus efficiently?

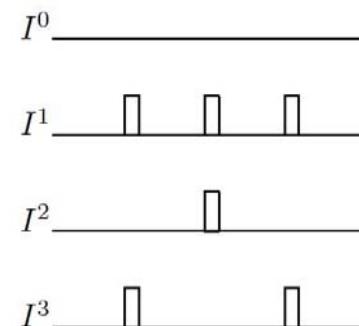
# Control: efficient refocusing

If all the qubits are coupled, expectation is that it is not possible, but if we have only two qubit coupling:



This is not efficient, instead use Hadamard matrices, (put a refocusing at each change of sign in a row)

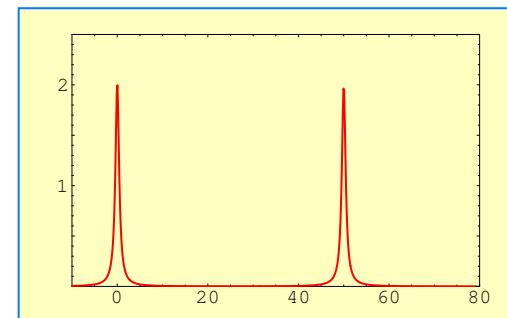
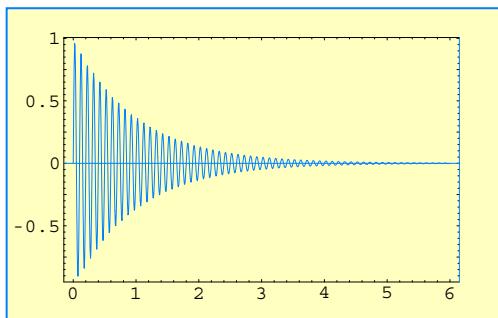
$$\begin{pmatrix} + & + & + & + \\ + & - & + & - \\ + & + & - & - \\ + & - & - & + \end{pmatrix}$$



# Measurement

For two spins, the magnetization  $M(t) = \text{Tr}[\rho(t)(I_-^1 + I_-^2)]$

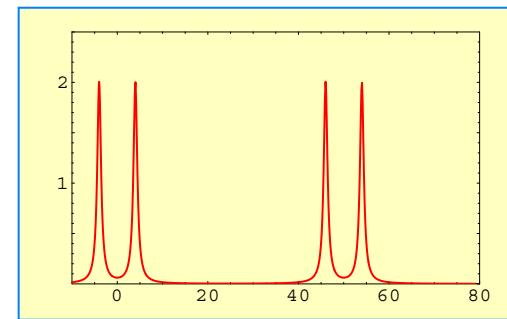
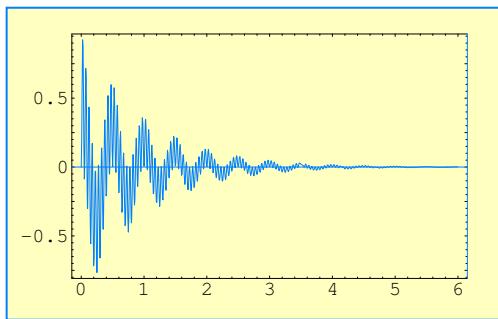
$$\rho(t) = e^{-it(\omega^1 Z_1 + \omega^2 Z_2)t} \rho(t_0) e^{it(\omega^1 Z_1 + \omega^2 Z_2)t}$$



The Fourier transform has a peak at the Larmor frequency. The integral of the peak gives us the scale of the matrix element, the width estimates  $T_2$ .

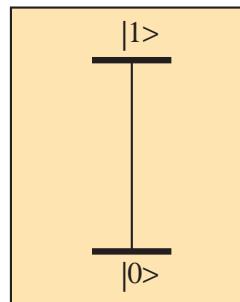
- In the presence of coupling,

$$\rho(t) = e^{-it(\omega^1 Z_1 + \omega^2 Z_2 + JZ_1 Z_2)} \rho(t_0) e^{it(\omega^1 Z_1 + \omega^2 Z_2 + JZ_1 Z_2)}$$

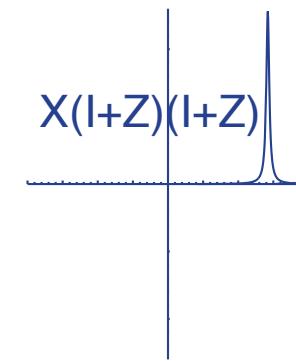
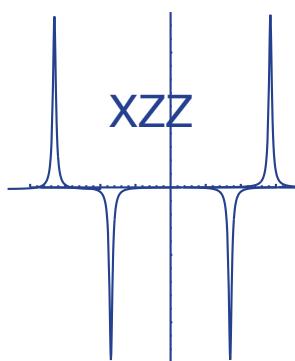
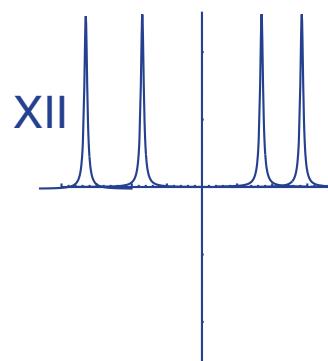
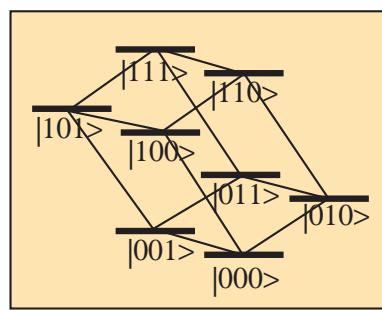
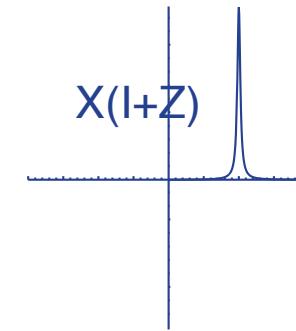
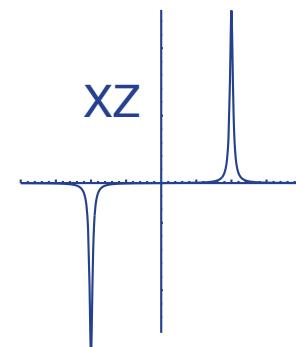
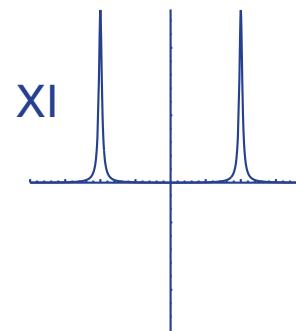
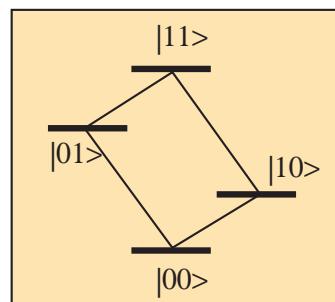


Coupling between qubits is seen has the splitting of the lines in two, corresponding to having the second qubit is in the state  $|0\rangle$  or  $|1\rangle$

# Interpretation of spectra



Observable is the transition  
 $|0\rangle\langle 1| + |1\rangle\langle 0|$  of a given spin



# Initial state (1)

The initial state is  $\rho = e^{-\beta H}/\text{Tr}e^{-\beta H}$  with  $\beta\omega_L \sim 10^{-5}$  implies

$$\rho \approx \frac{1}{N}(\mathbb{1} - \beta \sum_i \omega_i Z_i)$$

**Sorensen [6], Schulman and Vazirani [5]: concentrate polarization of the qubits.**  
**A 3 qubit example: if  $H = \omega(Z_1 + Z_2 + Z_3)$ , we can increase polarization by swapping the states  $|011\rangle \longleftrightarrow |100\rangle$**

$$\rho_{\text{thermal}}^d \approx \frac{\beta\omega}{8} \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix} \iff \rho_{\text{pol}}^d \approx \frac{\beta\omega}{8} \begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \end{pmatrix}$$

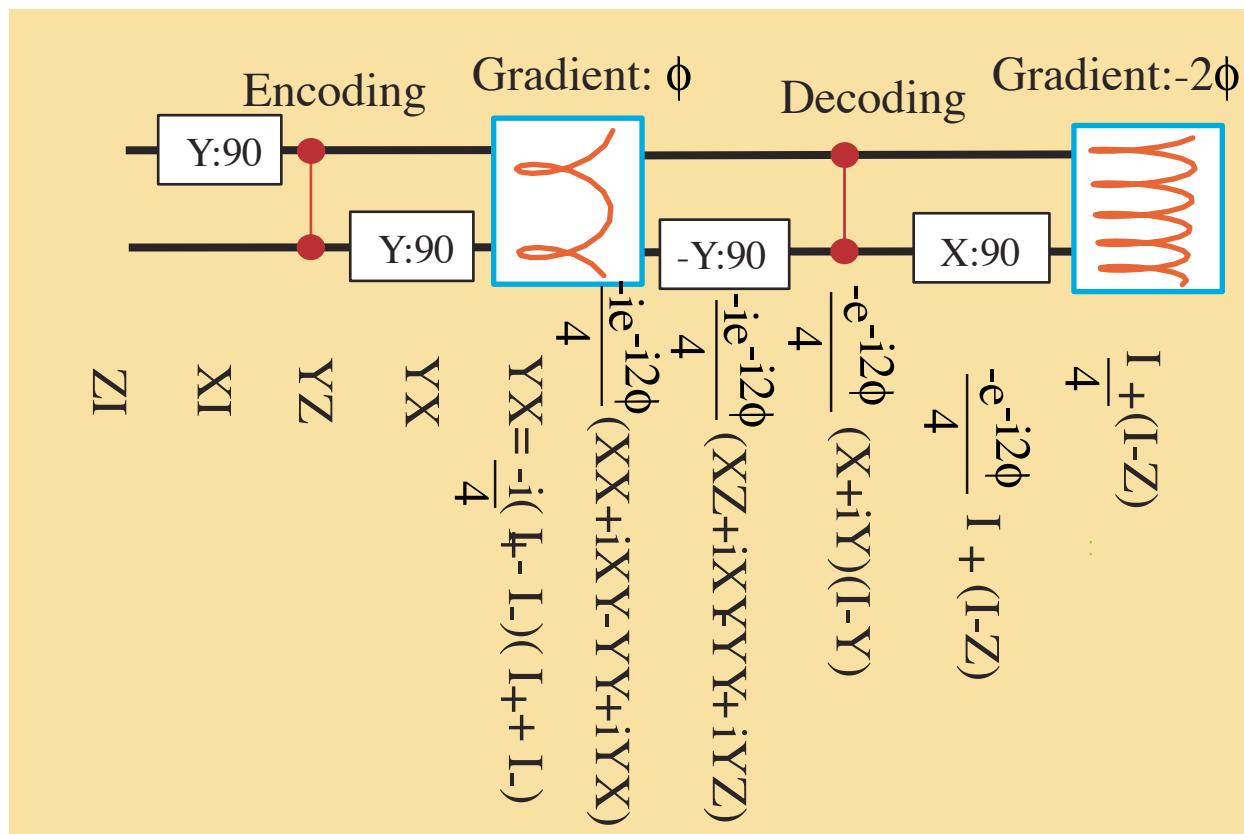
$$\bar{\rho}_{\text{pol}}^d = \text{Tr}\rho_{\text{pol}}^d \approx \frac{3}{4}\beta\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

# The initial state (2)

$$\rho = \frac{1}{Z} e^{-\beta H} \sim \frac{1}{Z} (\mathbb{1} - \beta H + \dots)$$

**Making a pseudo pure state** (Cory et al 1996, Gershenfeld et al. 1997)

$$\frac{1}{Z} (\mathbb{1} - \beta H) \rightarrow \frac{1}{Z} (\mathbb{1} - \frac{\beta \omega n}{2^n} |\Psi\rangle\langle\Psi|)$$



# Highly mixed state for QIP

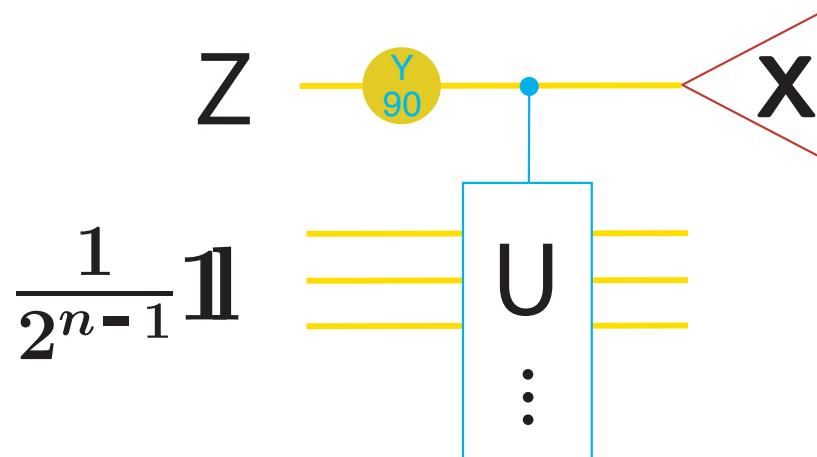
E. Knill & R.L. PRL81, 5672, 1998

$$\rho_i = \frac{1}{Z} e^{-\beta H} \approx \frac{1}{Z} (\mathbb{1} - \beta H + \dots)$$

Making a pseudo pure state on only one bit

$$\rho_i = \frac{1}{N} (\mathbb{1} - \frac{\omega}{kT} Z \otimes \mathbb{1} \otimes \dots)$$

and evolve with  $U_{\text{one bit}}$  described the circuit below, measuring  $X$  on the first qubit alone will give



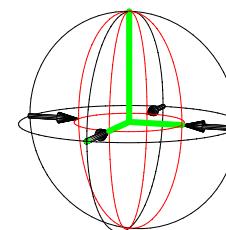
$$\text{Tr}[X_1 U_{\text{one bit}} \rho_i U_{\text{one bit}}^\dagger] = \frac{1}{2^{n-1}} \text{Re}(\text{Tr}[U])$$

# Noise

The strong magnetic field in the  $z$  direction, with some work to homogenize the magnetic in the  $X - Y$  direction reduces the number of parameters that describe the noise to three. The temperature,  $T_2$  and  $T_1$ .

$T_2$  describe the rate of decoherence (the randomization of the phase) which induce the decay of the off diagonal terms. It is caused by coupling to other spins or to the inhomogeneity of the magnetic field. It is a unital quantum operation, i.e. preserve the unit matrix.

$$\rho = \begin{pmatrix} a & b + ic \\ b - ic & 1 - a \end{pmatrix} \rightarrow \begin{pmatrix} a & (b + ic)e^{-t/T_2} \\ (b - ic)e^{-t/T_2} & 1 - a \end{pmatrix}$$



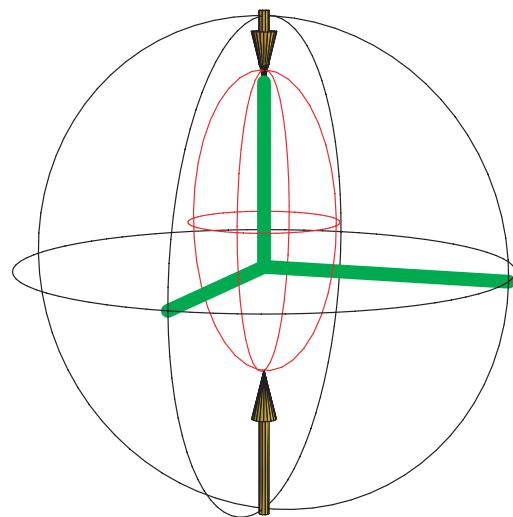
$T_2$  is of the order off seconds in liquid state NMR.

**Relaxation to thermal equilibrium is given at a rate called  $T_1$ . It describe the interaction with the “lattice”.**

**The evolution of a family of isolated spin in pure states evolve as:**

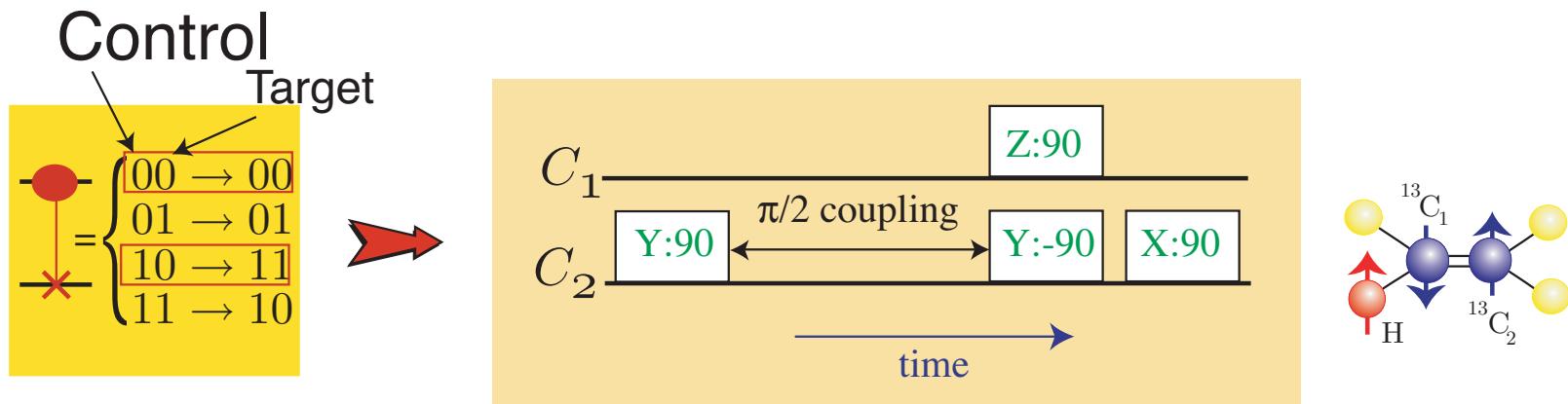
$$\begin{aligned}\rho &= \begin{pmatrix} \rho_{00}^i & \rho_{01}^i \\ \rho_{10}^i & \rho_{11}^i \end{pmatrix} \\ \rightarrow \quad \rho &= \begin{pmatrix} \rho_{00}^{\text{eq}}(1 - e^{t/T_1}) + \rho_{00}^i e^{-t/T_1} & \rho_{01}^i e^{-t/2*T_1} \\ \rho_{10}^i e^{-t/2*T_1} & \rho_{11}^{\text{eq}}(1 - e^{t/T_1}) + \rho_{11}^i e^{-t/T_1} \end{pmatrix}\end{aligned}$$

**with  $\rho_{00}^{\text{eq}} = e^{\beta\omega}/(e^{\beta\omega} + e^{-\beta\omega})$  and  $\rho_{11}^{\text{eq}} = e^{-\beta\omega}/(e^{\beta\omega} + e^{-\beta\omega})$**



**$T_1$  for liquid state NMR is of the order of seconds to tens of seconds.**

# Control-Not from NMR gates

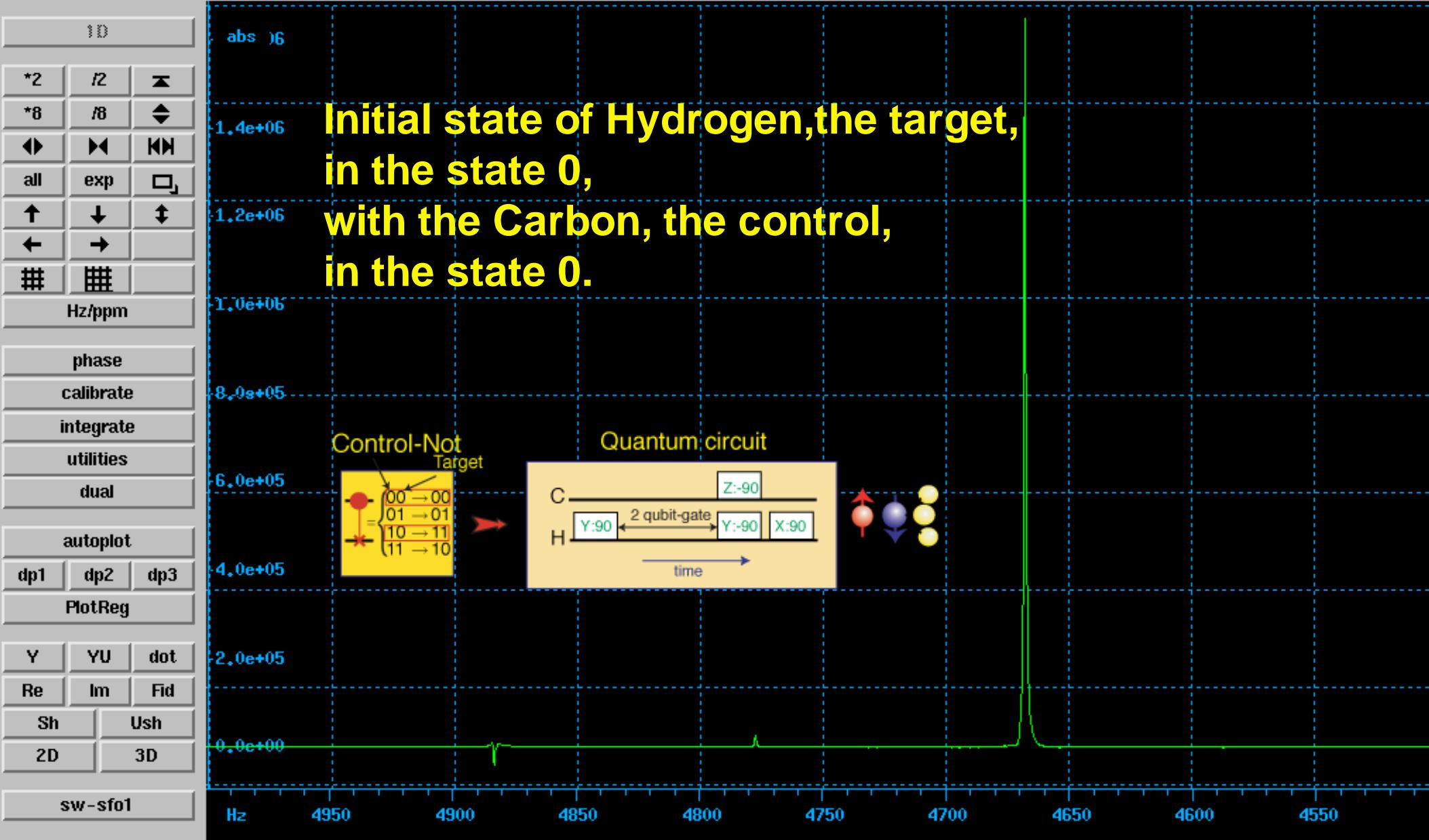


A control-not is implemented by combining one bit gates and a single two qubit gate.  $C_1$  is the control and  $C_2$  the target.  
We can translate these gates into the spectrometer language.

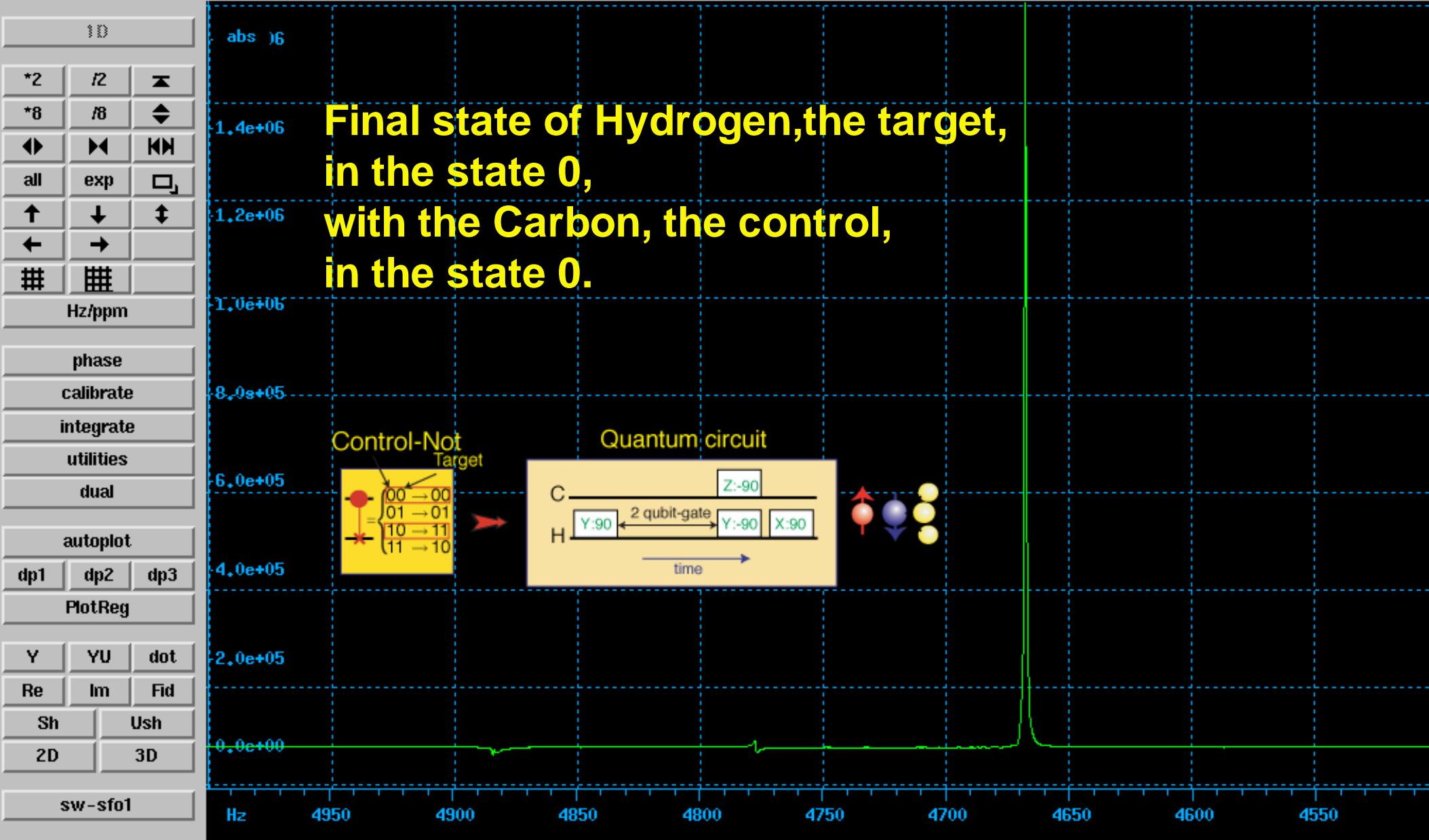
Pulse sequence

```
(C2_-90:sp9 ph13 ) :f1  
3u  
3u ipp13  
0.71365m  
8u  
8u  
(C2_-90:sp9 ph19) :f1  
6u ipp15 ipp19  
8u  
(C2_-90:sp9 ph20) :f1  
6u ipp15 ipp20
```

# Control-Not at the spectrometer



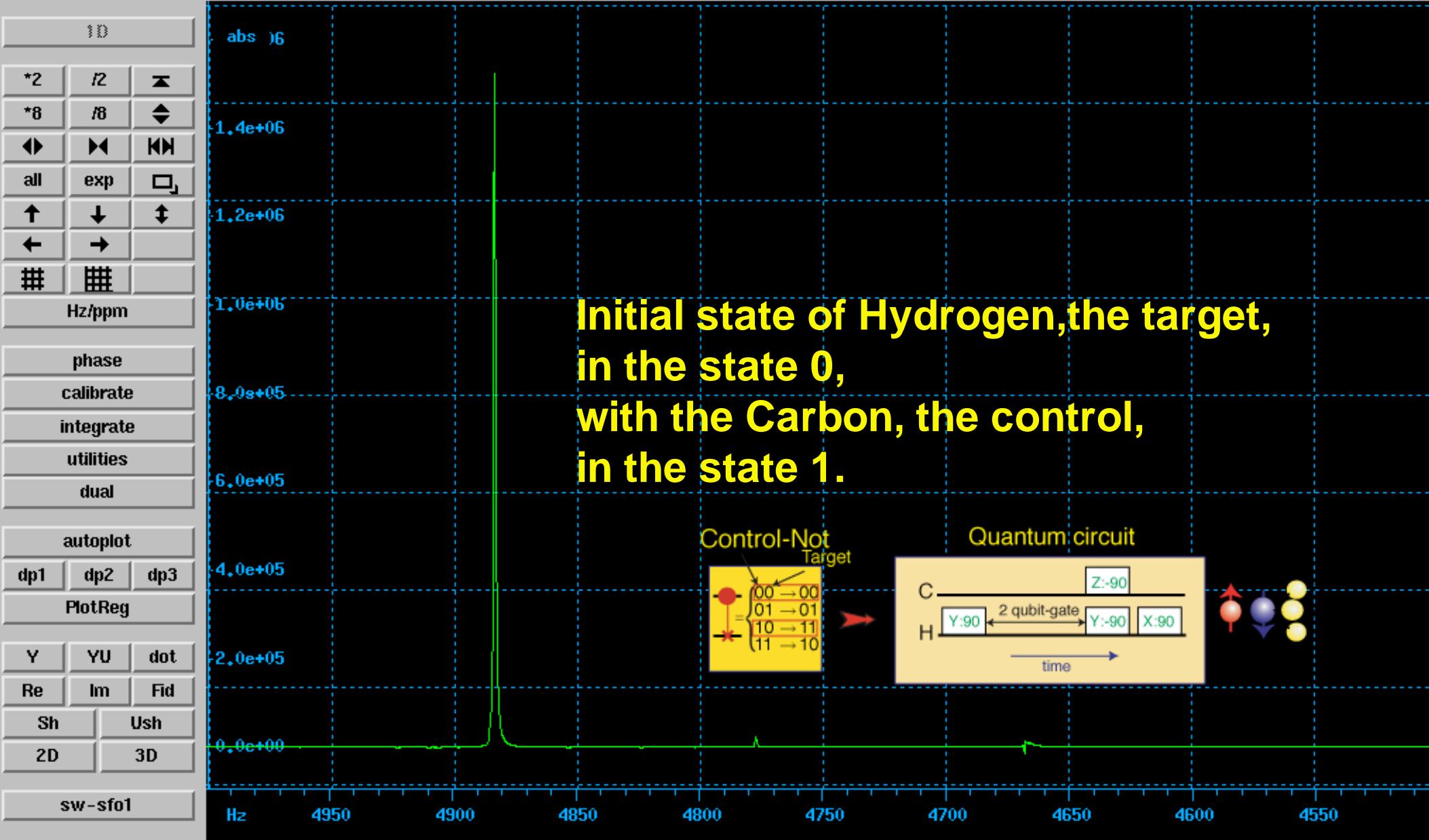
# Control-Not at the spectrometer



]

iexpno.exe : finished

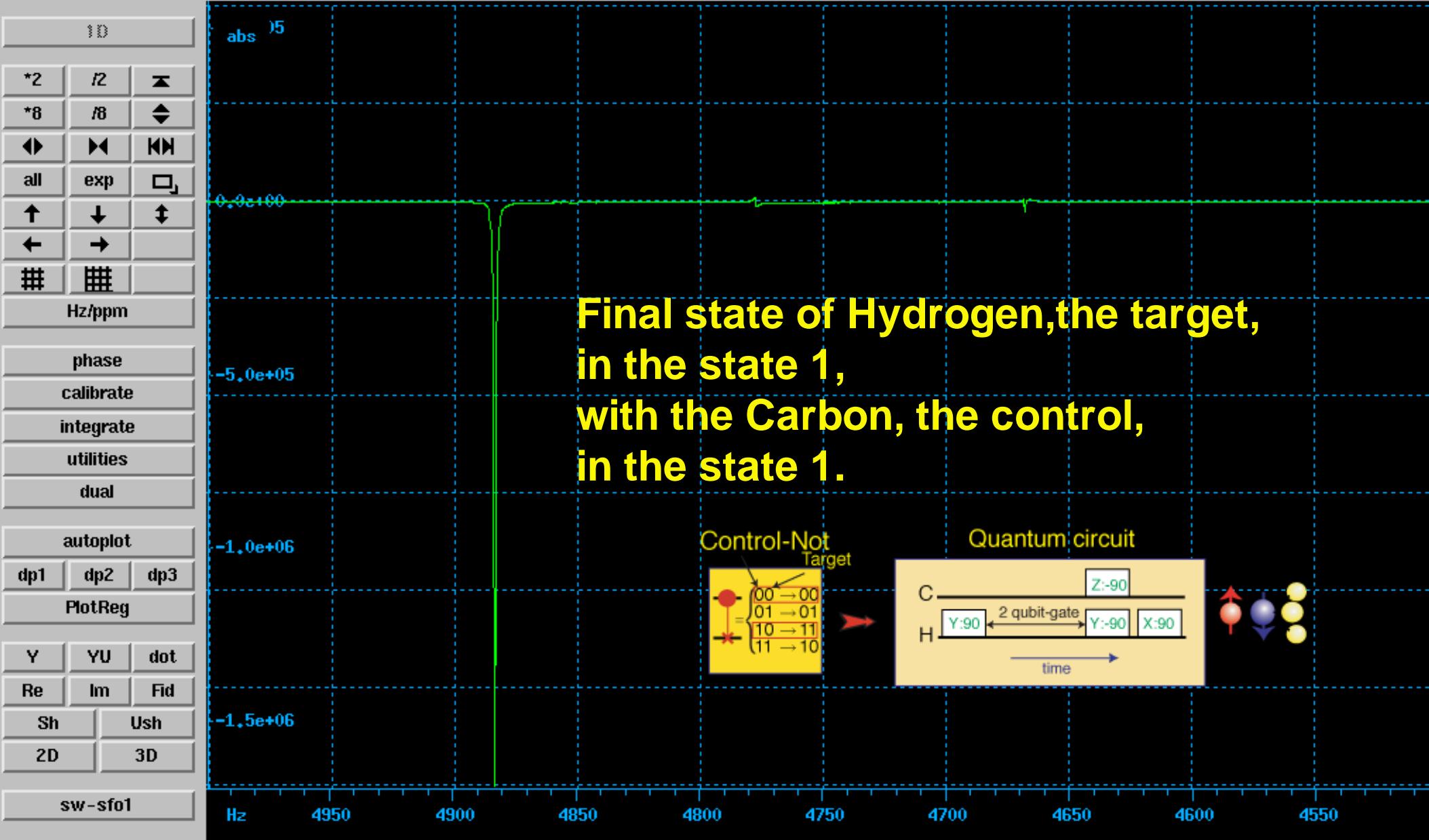
# Control-Not at the spectrometer



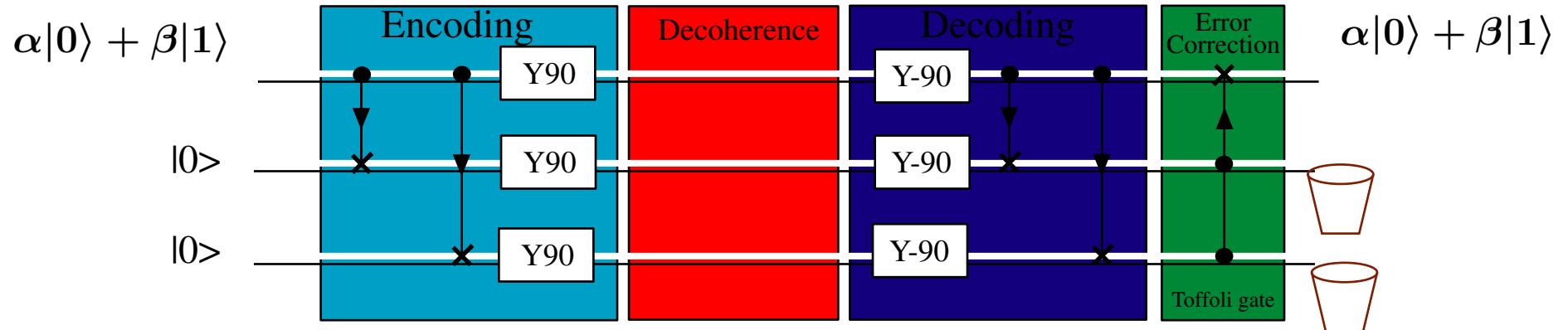
&gt;

iexpno.exe : finished

# Control-Not at the spectrometer



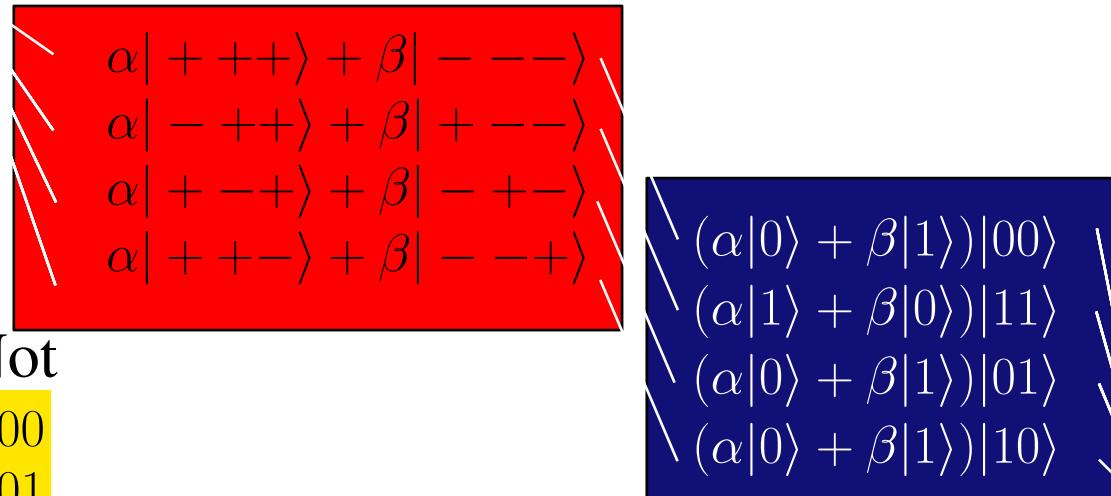
# 3 qubit code for phase errors



$\alpha|0\rangle + \beta|1\rangle$

Errors:  $+$   $\rightarrow$   $-$

$-$   $\rightarrow$   $+$



Control-Not

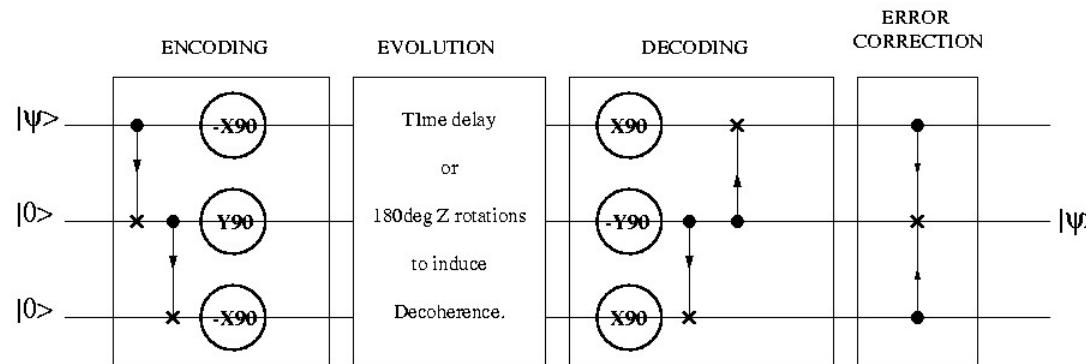
$$\begin{matrix} \bullet \\ \downarrow \\ \times \end{matrix} = \begin{cases} 00 \rightarrow 00 \\ 01 \rightarrow 01 \\ 10 \rightarrow 11 \\ 11 \rightarrow 10 \end{cases}$$

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$$

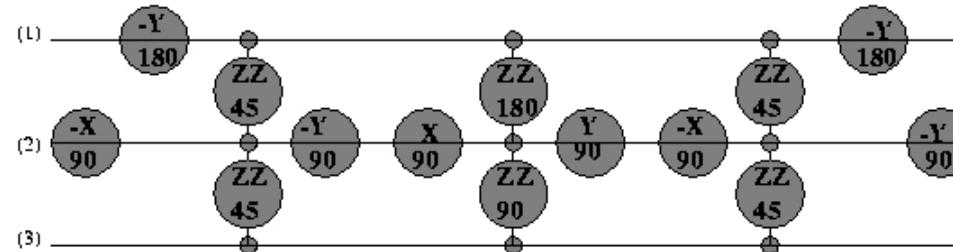
$$(\alpha|0> + \beta|1>) \otimes \begin{cases} 00 \\ 11 \\ 01 \\ 10 \end{cases} \sim 1 - 3\gamma^2$$

# Phase QEC NMR circuit

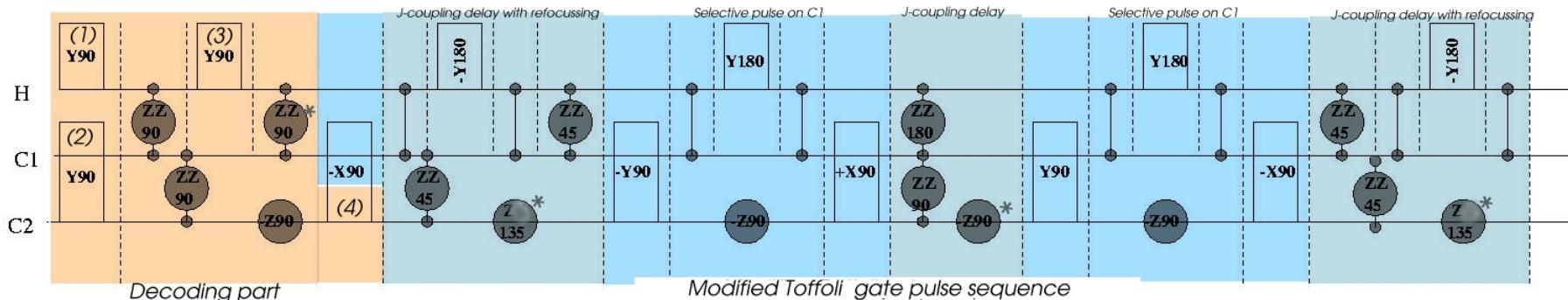
NMR implementation of the decoding and error correction:



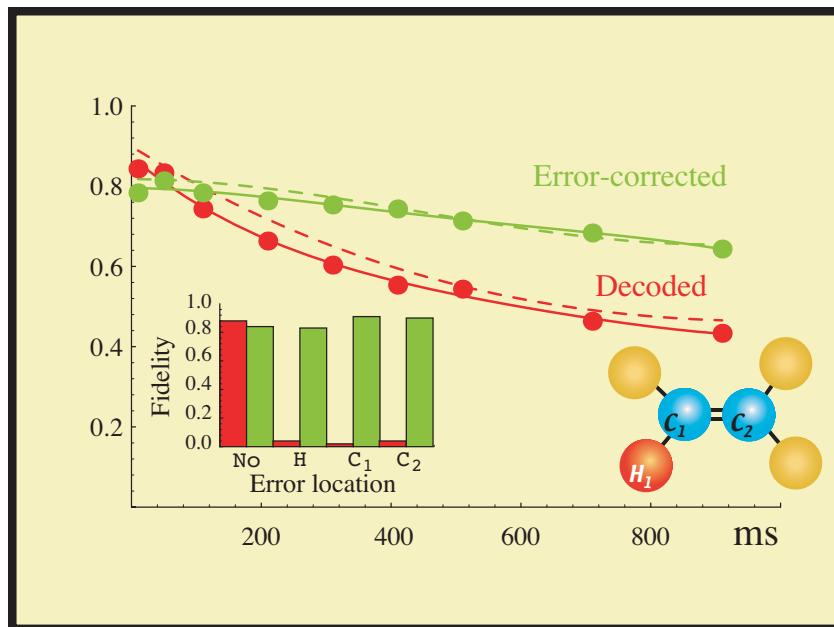
Toffoli gate:



and the full decoding and Toffoli, including some optimization



# Experimental results

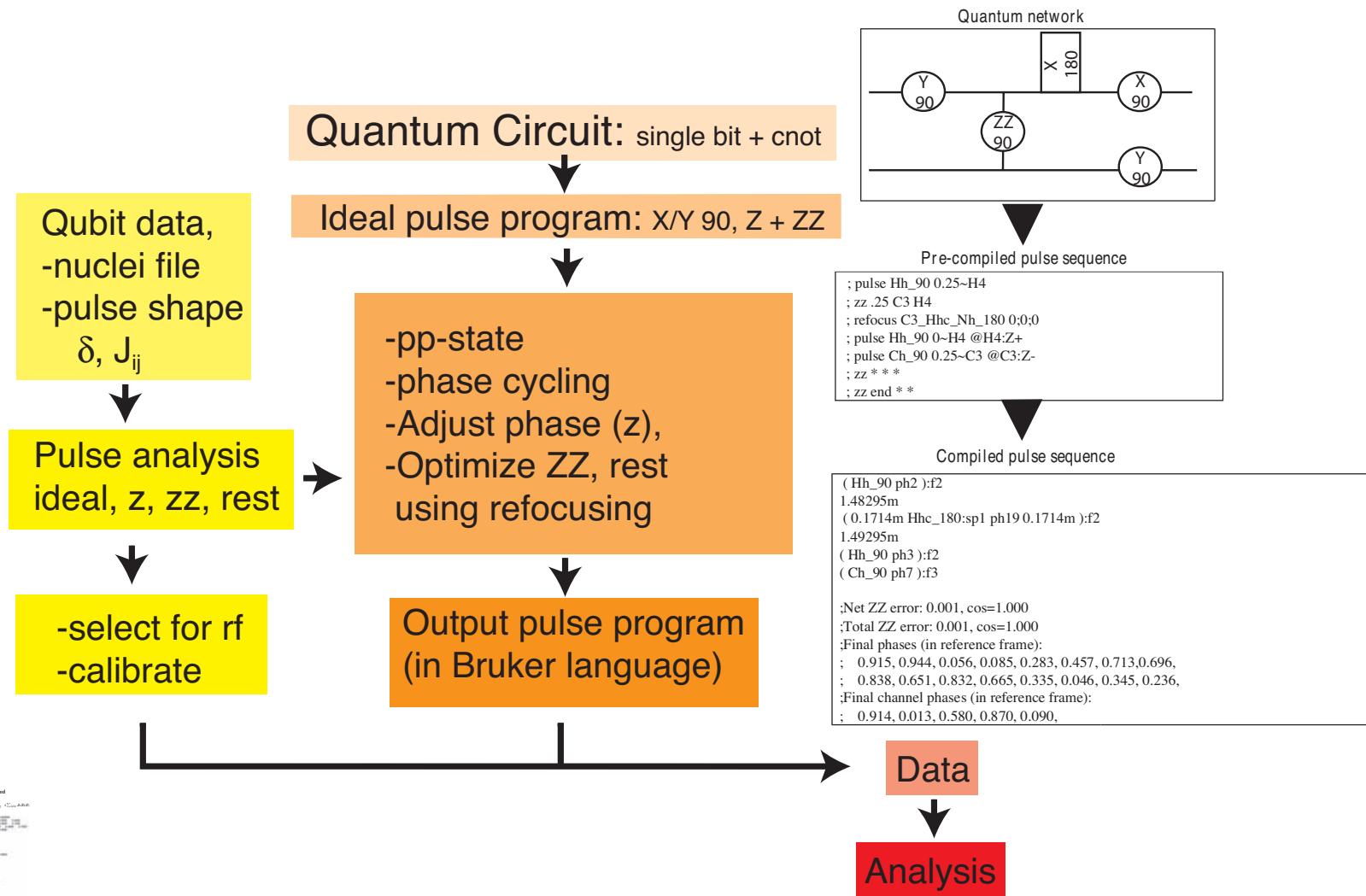


The demonstration of quantum error correction is in the shape of the green curve which does not have the first order error. The curve is much flatter than the red one.

Experimental Quantum Error Correction:  
D. G. Cory, M. D. Price, W. Maas, E. Knill,  
R. Laflamme, W. H. Zurek, T. F. Havel and  
S. S. Somaroo, PRL 81, 2152, 1998

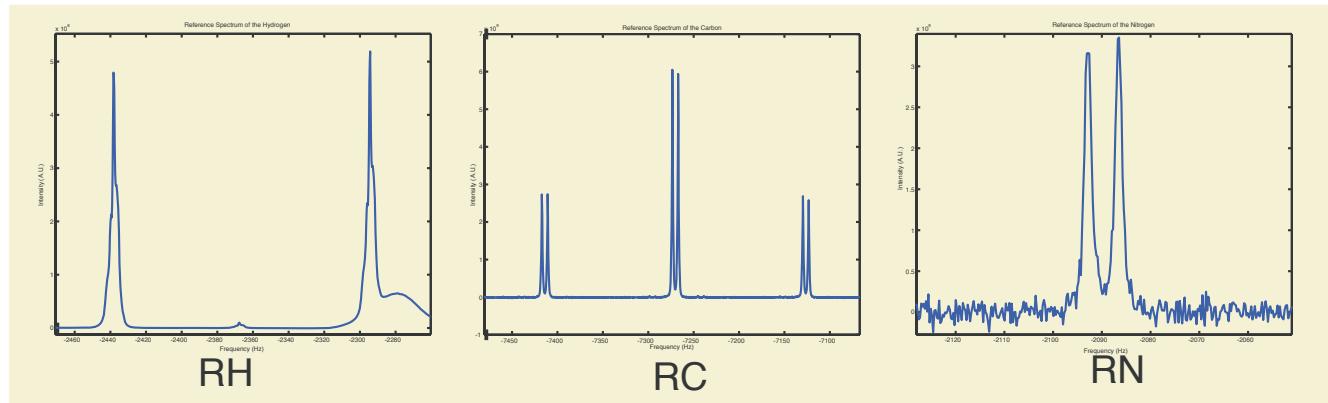
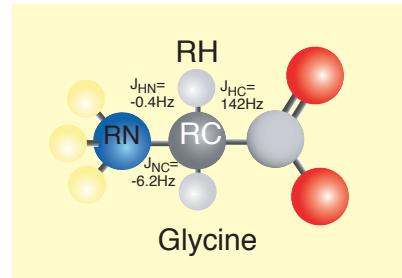
# A quantum compiler

As we increase the number of qubits, we need to automate many tasks such as the re-focusing schemes and also deal systematically with errors that can be partially corrected.



# Pulse calibration

- Decide which pulses are required:  
soft or hard pulse  
90° and 180°
- Use a molecule with simpler spectra:



# Spin half selection

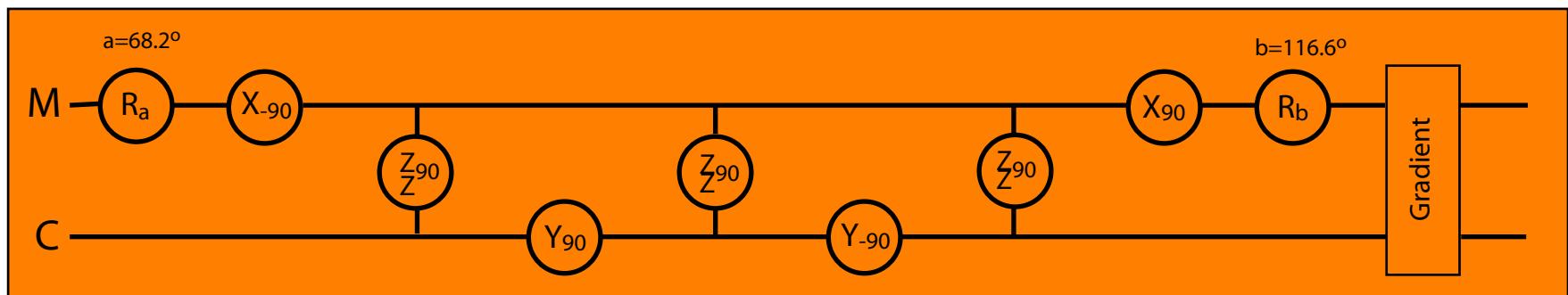
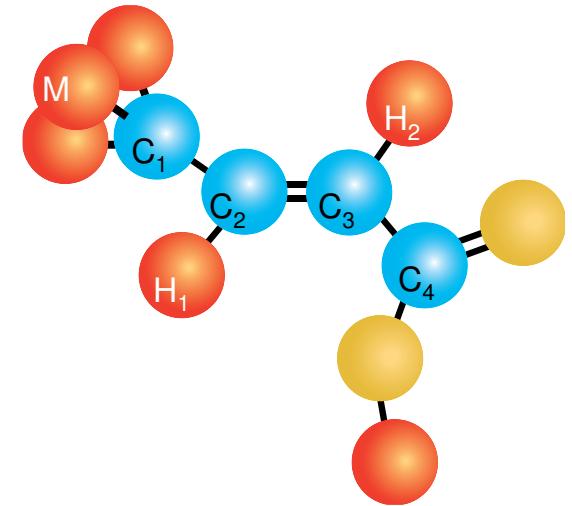
Projection on the spin 1/2

$$P_{1/2} = \mathbb{1} - P_{3/2}$$

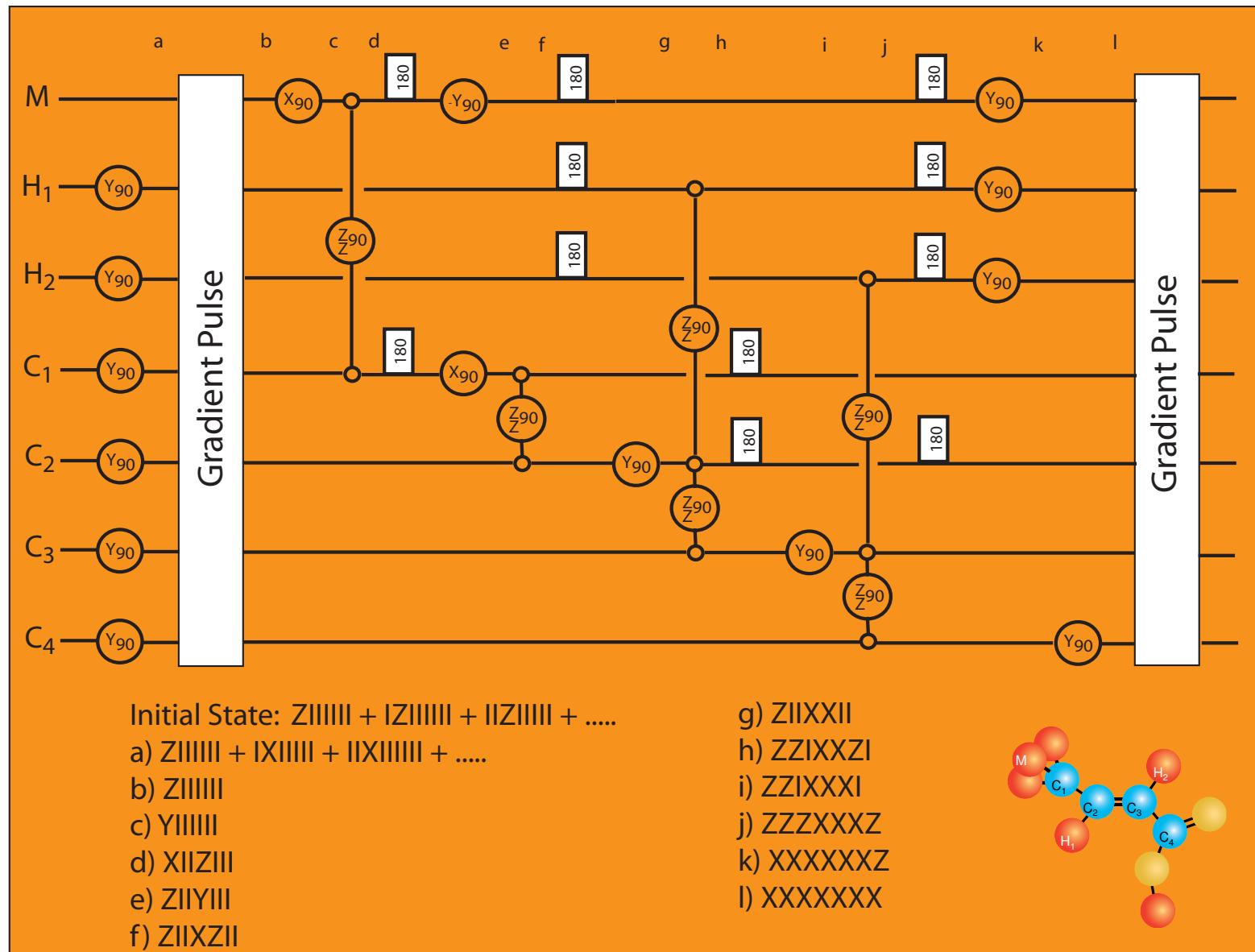
$$= \mathbb{1} - [ |3/2, 3/2\rangle + |3/2, 1/2\rangle + |3/2, -1/2\rangle + |3/2, -3/2\rangle ]$$

in term of operators we have

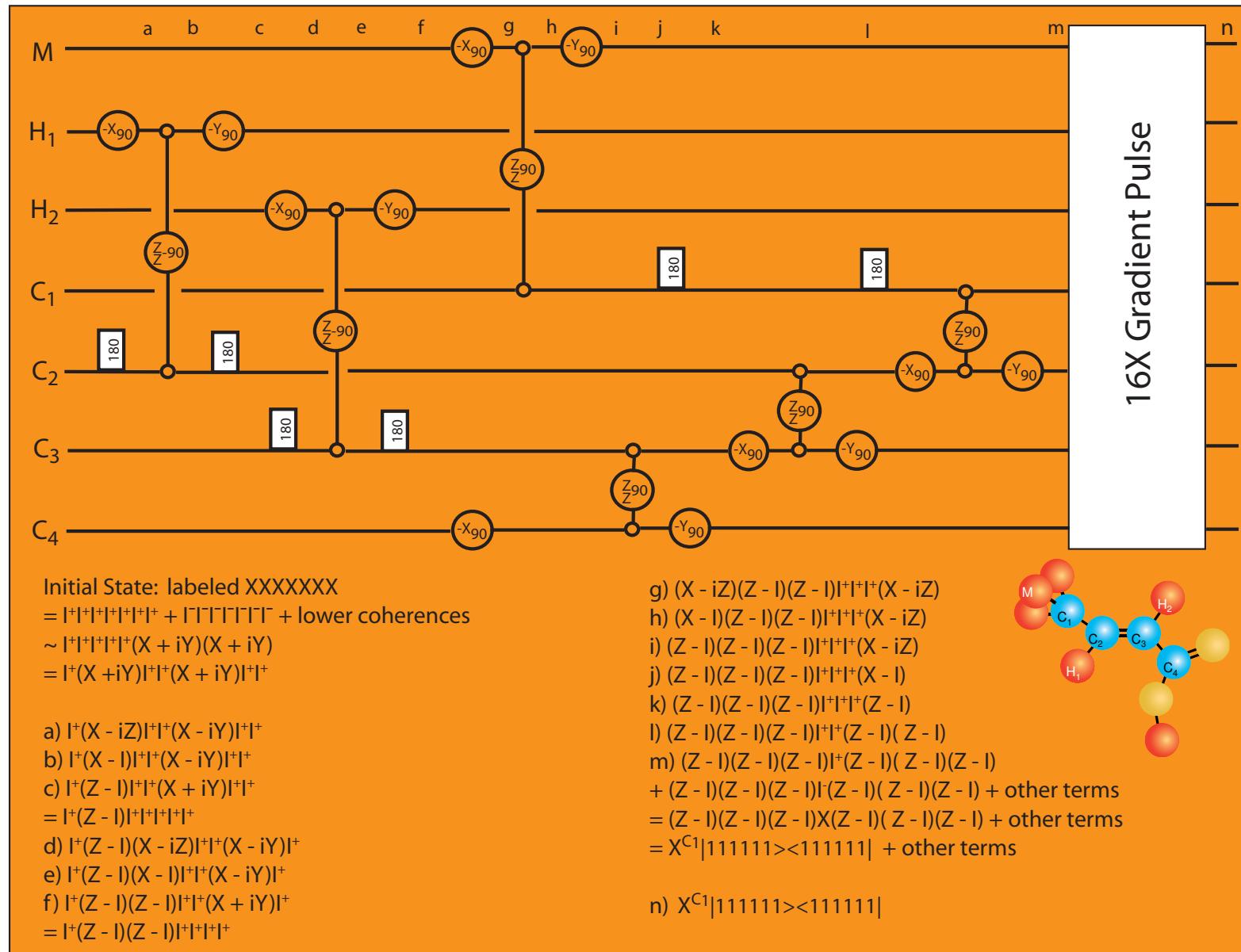
$$P_{1/2} = [\frac{1}{2}\mathbb{1}\mathbb{1}\mathbb{1} - \frac{1}{6}[(\mathbb{1}XX) + (\mathbb{1}YY) + (\mathbb{1}ZZ)]]$$



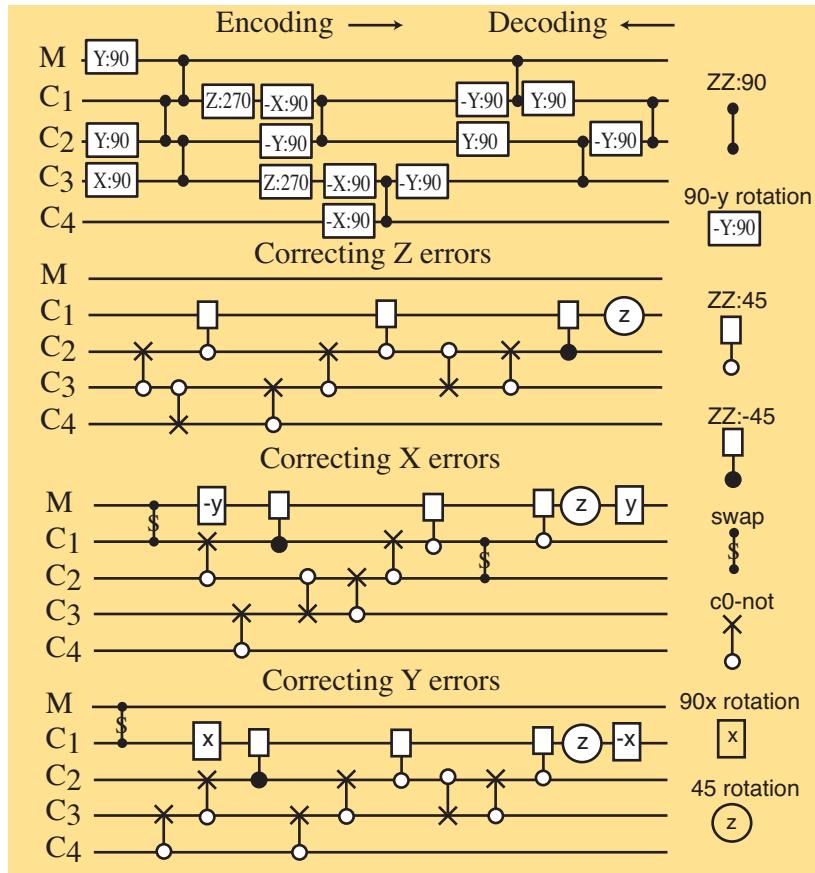
# PP state for crotonic acid: encoding



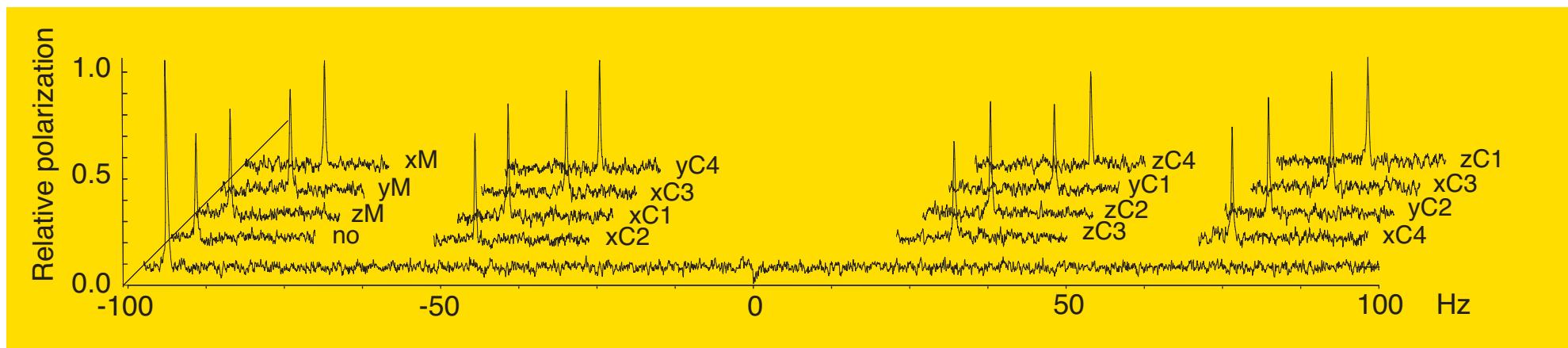
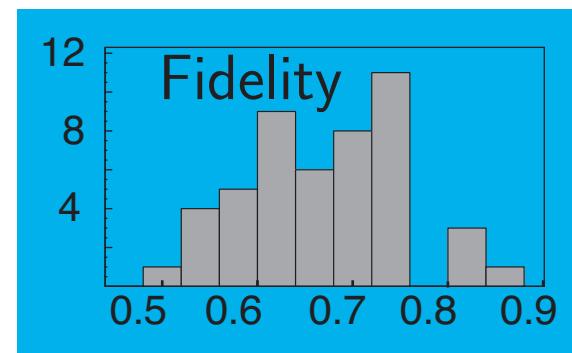
# PP state for crotonic acid: decoding



# 5 bit quantum error correcting code

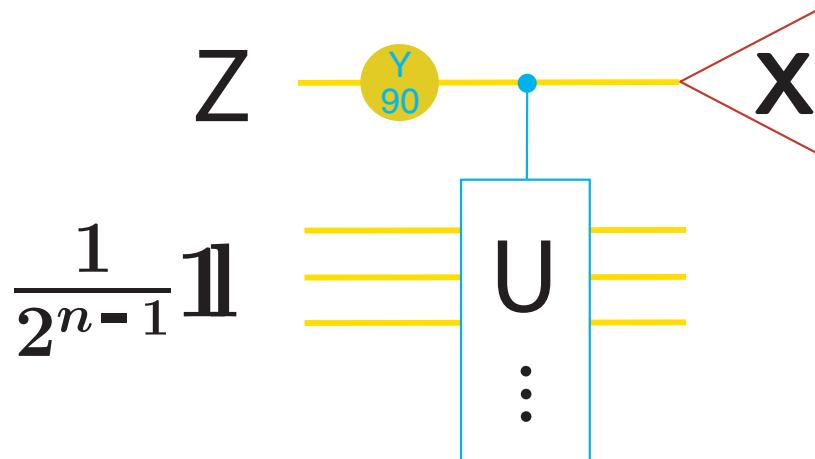


**Implementation of the 5 bit code with the stabilizer  $Z^2Y^3Y^4X^5$ ,  $Z^1Y^2Y^3X^4$ ,  $Y^2Z^3Z^4Z^5$  and  $X^1Z^2X^3Z^4$ , including decoding and error correction for a basis of 1 qubit errors [1].**



# The power of one qubit

We have seen that the circuit below can be powerful computationnaly



$$\text{Tr}[X_1 U_{\text{one bit}} \rho_i U_{\text{one bit}}^\dagger] = \frac{1}{2^{n-1}} \text{Re}(\text{Tr}[U])$$

Are there any interesting  $U$ ?

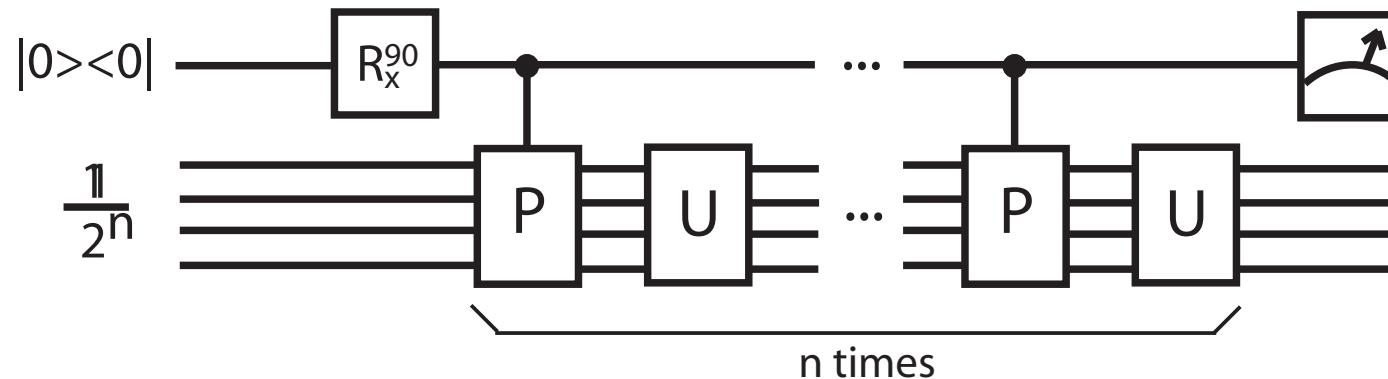
It is possible to characterize complex dynamics. In reference [3] it was suggested that the average fidelity decay of the state can be used to characterise if a unitary operator  $U$  has symmetries (regular system) or not (quantum chaotic) using where we evolve under a unitary evolution  $UP$  where  $U$  is characteristic of the evolution  $U$  of a perturbation  $P$

$$F_n(\psi) = \left| \langle \psi | (U^n)^\dagger U_p^n | \psi \rangle \right|^2$$

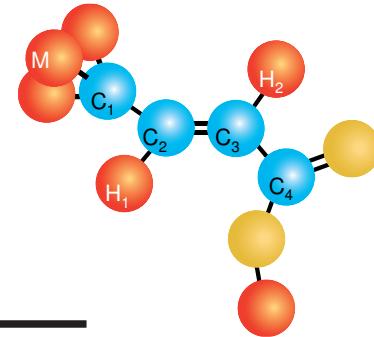
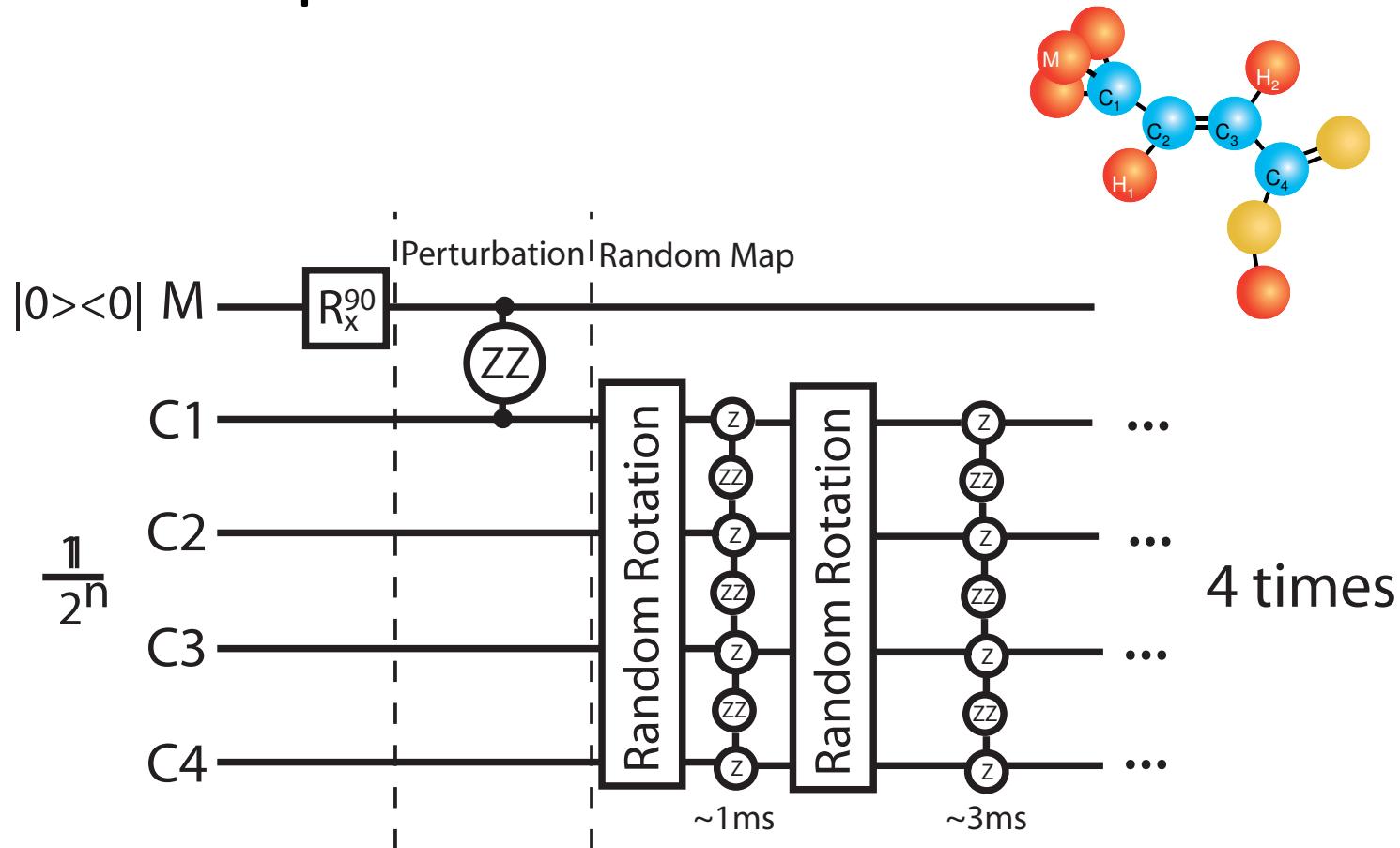
is given by

$$\overline{F}_n = \frac{\left| \text{Tr} \left[ (U^n)^\dagger (PU)^n \right] \right|^2 + N}{N^2 + N}.$$

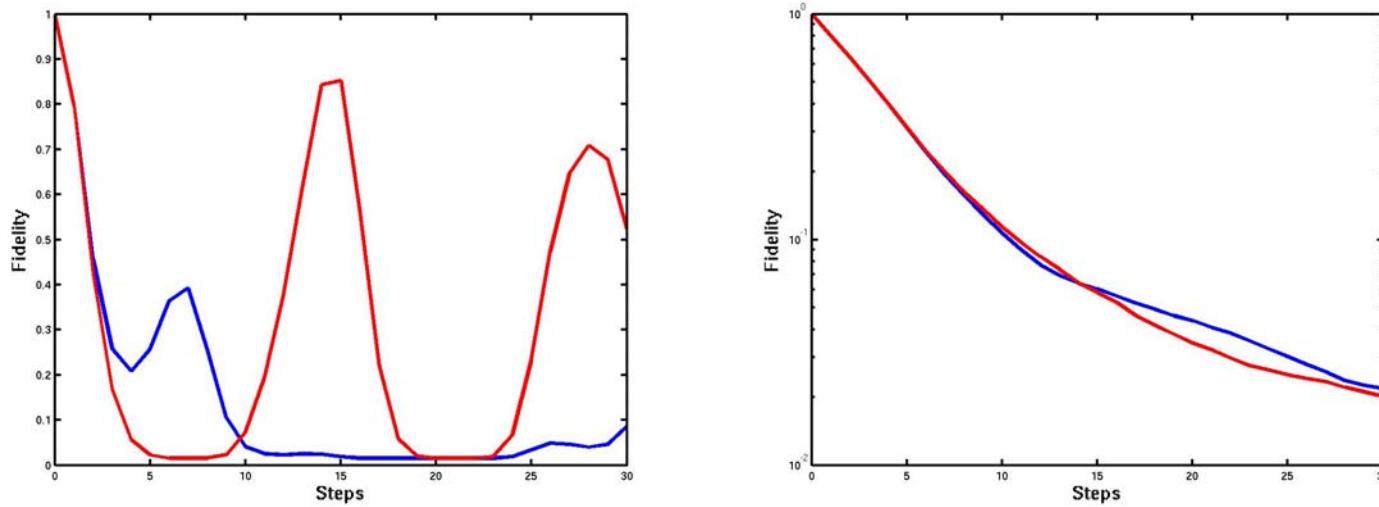
A simplified circuit to evaluate this is given by (noting that the control on the  $U$  can be dropped without changing the circuit):



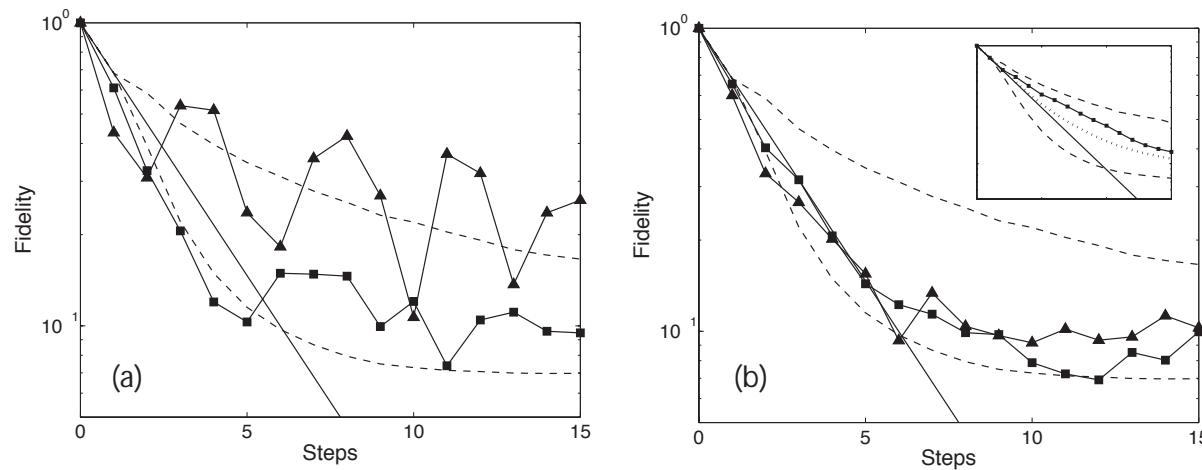
The circuit can be implemented in crotonic acid



The diagrams below give the behavior of regular and chaotic evolution:



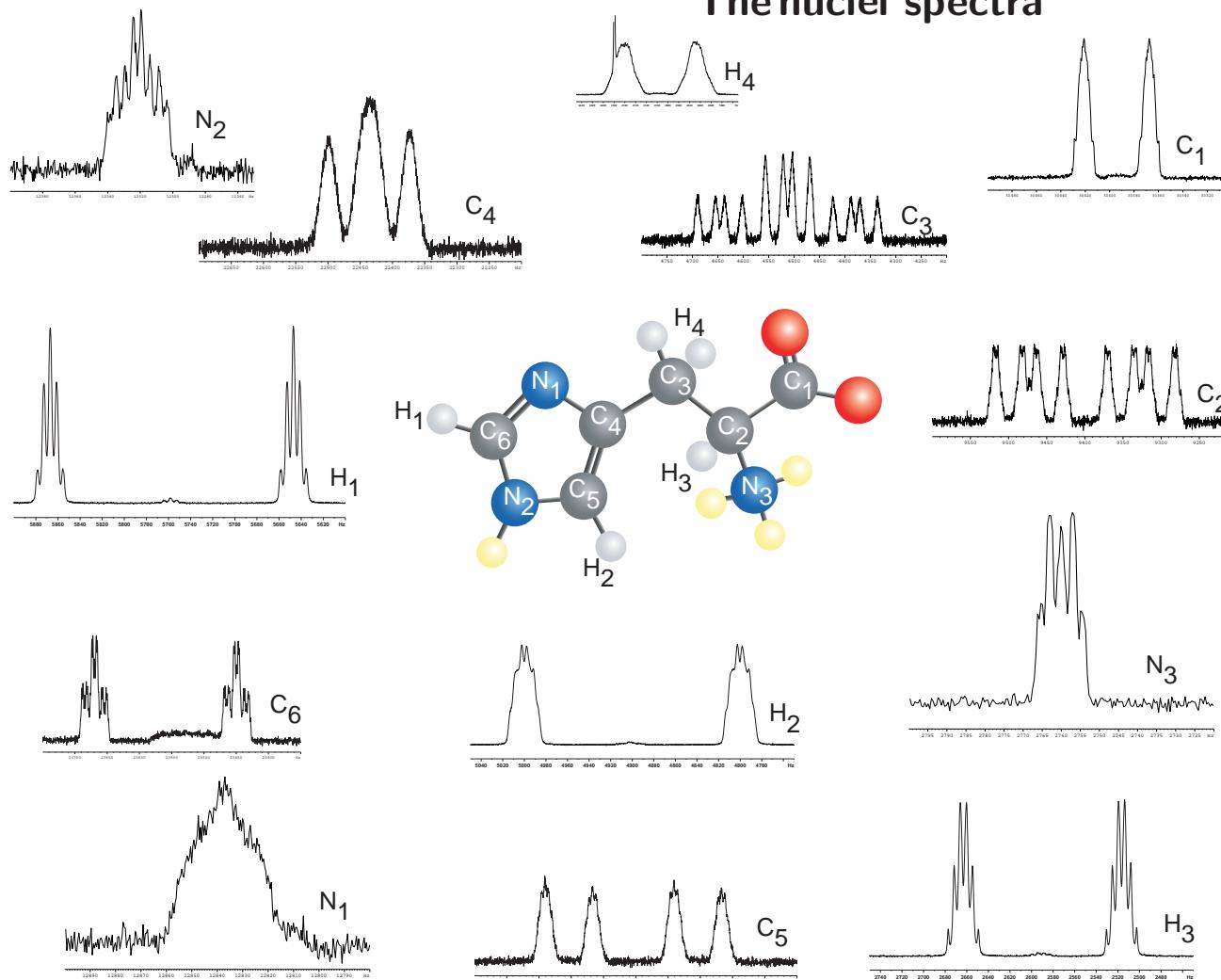
and experimentally we obtain:



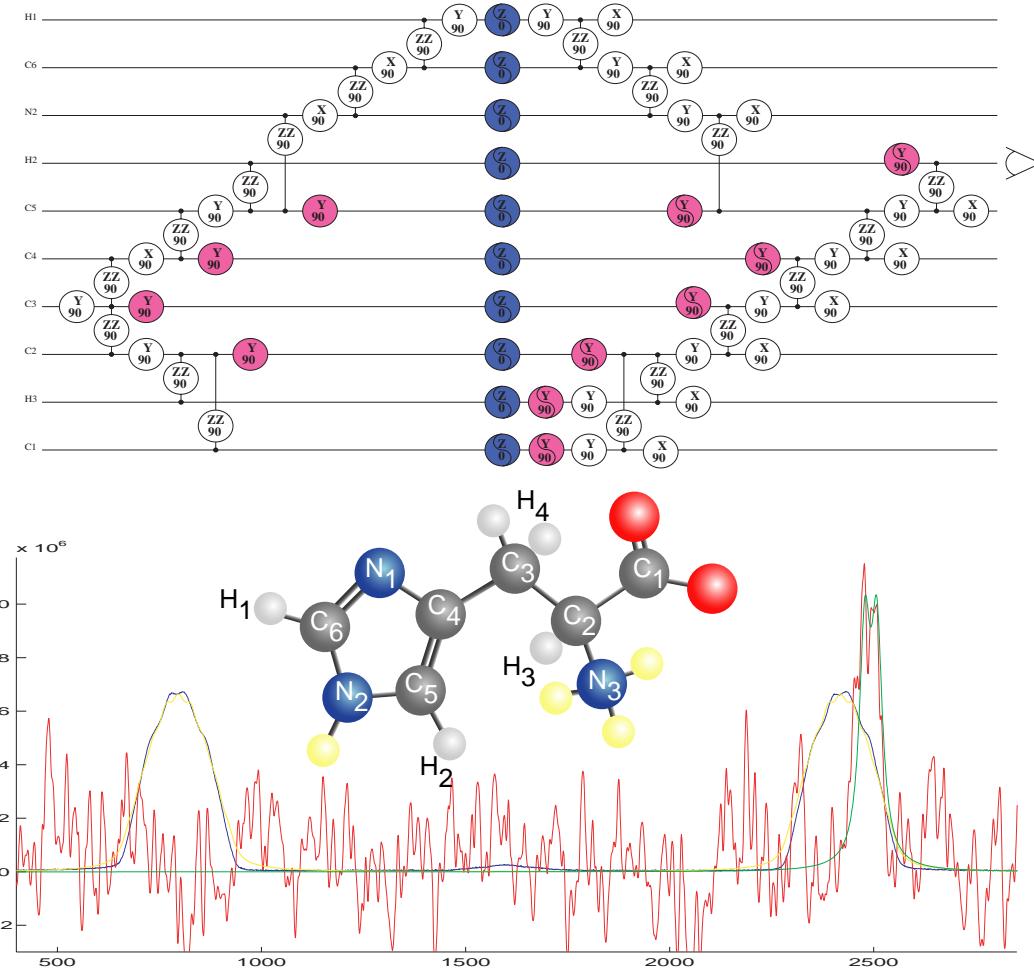
For details see [4]

# QIP with histidine

The nuclei spectra



# A ten qubits cat-state in histidine



# References

- [1] E. Knill, R. Laflamme, R. Martinez, and C. Negrevergne. Implementation of the five qubit error correction benchmark. *Phys. Rev. Lett.*, 86:5811–5814, 2001.
- [2] R. Laflamme, E. Knill, D. Cory, E. M. Fortunato, T. Havel, C. Miquel, R. Martinez, C. Negrevergne, G. Ortiz, M. A. Pravia, S. Sinha, R. Somma, and L. Viola. Introduction to NMR quantum information processing. *Los Alamos Science*, (27):226–259, 2001. quant-ph/0207172.
- [3] D. Poulin, R. Blume-Kohout, R. Laflamme, and H. Ollivier. Exponential speed-up with a single bit of quantum information: Testing the quantum butterfly effect. *Phys. Rev. Lett.*, 92:177906, 2004.
- [4] C. Ryan and R. Laflamme. Characterization of complex quantum dynamics with a scalable nmr information processor. *Phys. Rev. Lett.*, 95:250502, 2005.
- [5] L. J. Schulman and U. Vazirani. Scalable NMR quantum computation. In *Proceedings of the 31th Annual ACM Symposium on the Theory of Computation (STOC)*, pages 322–329, El Paso, Texas, 1998. ACM Press.
- [6] O. W. Sørensen. Polarization transfer experiments in high-resolution NMR spectroscopy. *Prog. Nucl. Mag. Res. Spect.*, 21:503–569, 1989.