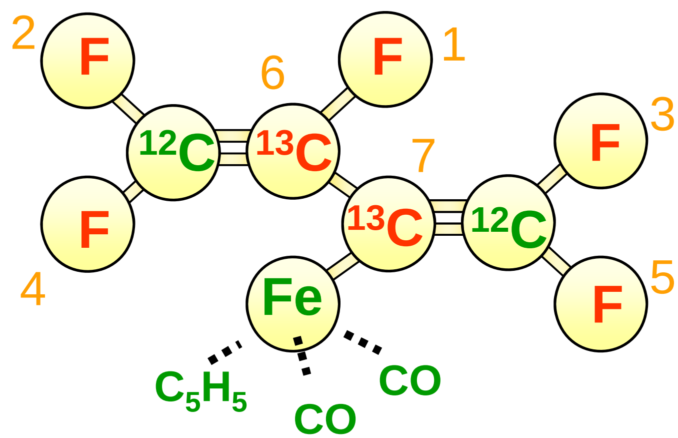
NMR Quantum Computing

Slides courtesy of **Lieven Vandersypen**
Then: IBM Almaden, Stanford University
Now: Kavli Institute of NanoScience, TU Delft

with some annotations by Andreas Wallraff.

How to factor 15 with NMR?

perfluorobutadienyl
iron complex



red nuclei are
qubits: F, ^{13}C

Goals of this lecture

Survey of NMR quantum computing

- Principles of NMR QC
- Techniques for qubit control
- State of the art
- Future of spins for QIPC
- Example: factoring 15

NMR largely satisfies the DiVincenzo criteria

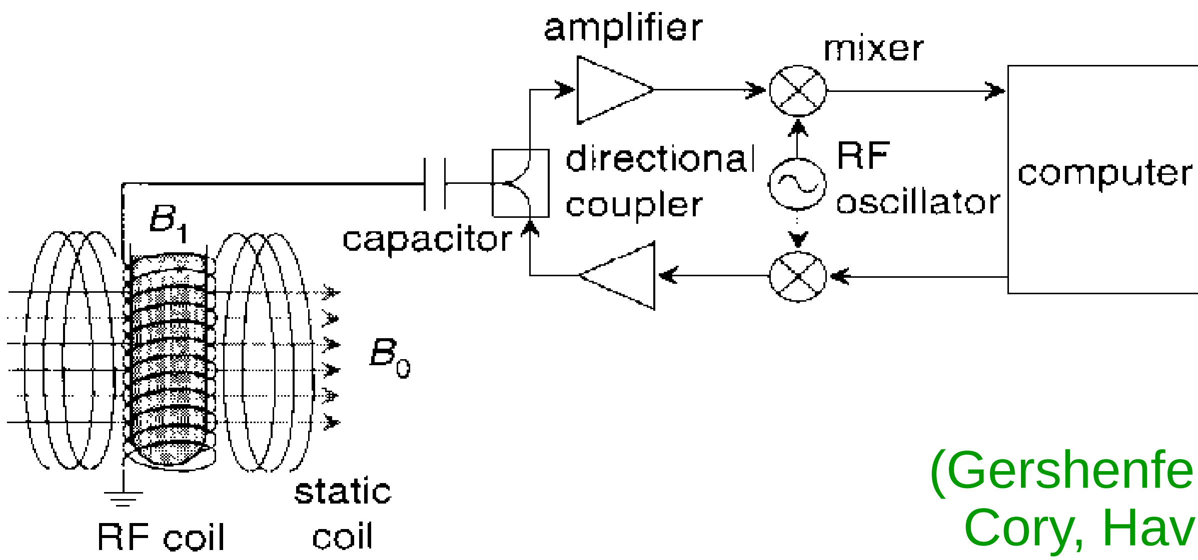
✓ Qubits: nuclear spins ½ in B_0 field (↑ and ↓ as 0 and 1)

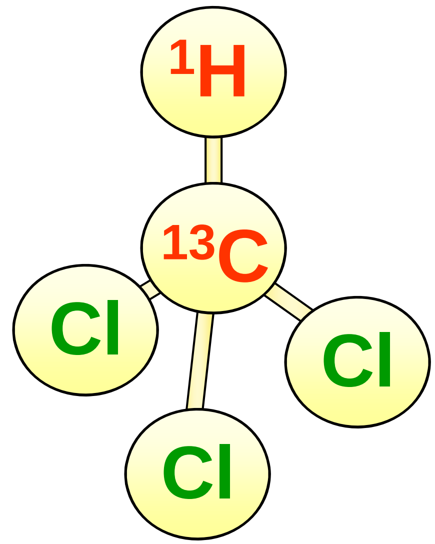
✓ Quantum gates: RF pulses and delay times

(✓) Input: Boltzman distribution (room temperature)

✓ Readout: detect spin states with RF coil

✓ Coherence times: easily several seconds

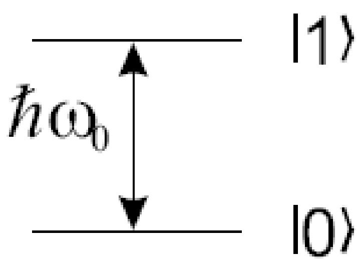


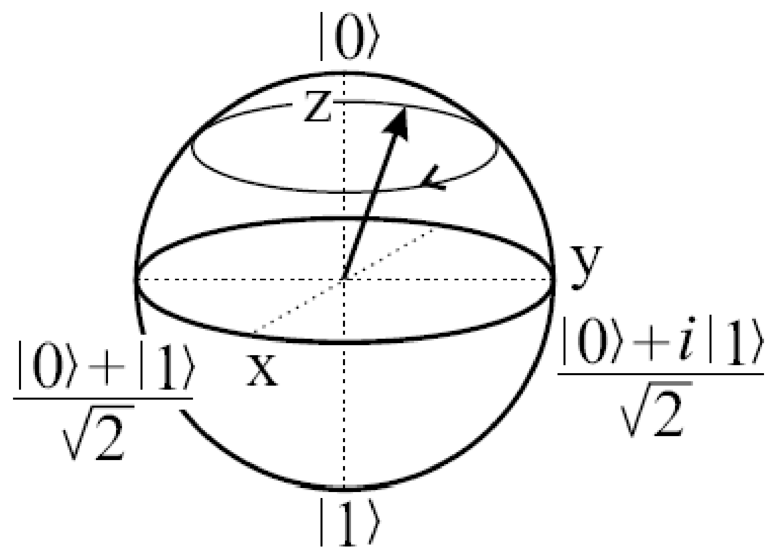


(Gershenfeld & Chuang 1997,
Cory, Havel & Fahmi 1997)

Nuclear spin Hamiltonian
Single spin

$$\mathcal{H}_0 = -\hbar\gamma B_0 I_z = -\hbar\,\omega_0\, I_z = \begin{bmatrix} -\hbar\omega_0/2 & 0 \\ 0 & \hbar\omega_0/2 \end{bmatrix}$$





angular momentum: $\vec{L} = \hbar \vec{I}$

magnetic moment: $\vec{M} = \gamma \hbar \vec{I}$

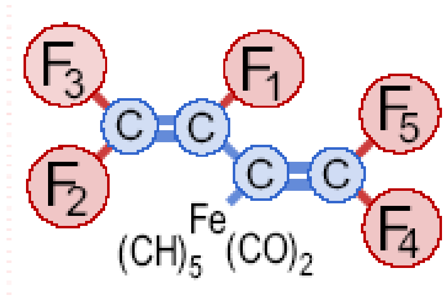
energy: $H_0 = -\vec{M} \cdot \vec{B}_0$

gyromagnetic (g-)factor: γ

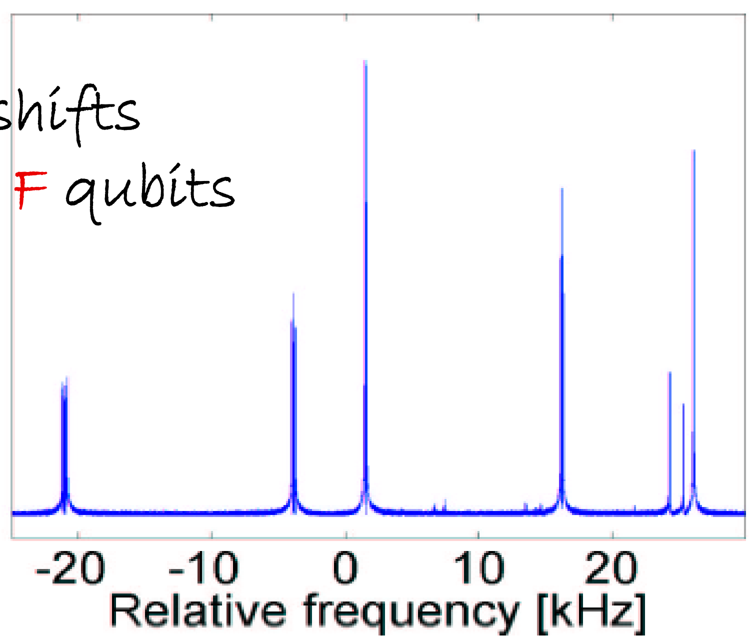
Nuclear spin Hamiltonian
Multiple spins

without qubit/qubit coupling

$$\mathcal{H}_0 = -\sum_{i=1}^{n} \hbar\,(1-\tilde{\sigma}_i)\gamma_i B_0\, I_z^i = -\sum_{i=1}^{n} \hbar\,\omega_0^i\, I_z^i$$



chemical shifts of the five F qubits



	MHz	
^{1}H	500	~ 25 mK
^{13}C	126	
^{15}N	-51	
^{19}F	470	
^{31}P	202	

(at 11.7 Tesla)

qubit level separation

Hamiltonian with RF field
single-qubit rotations

$$\overset{\sigma_z}{}\qquad\overset{\sigma_x}{}\qquad\overset{\sigma_y}{}$$

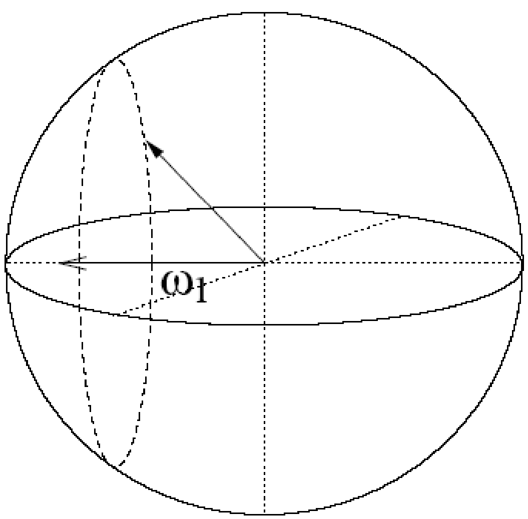
$$\mathcal{H} = -\hbar\,\omega_0\, I_z - \hbar\omega_1 \left[\cos(\omega_{rf} t + \phi) I_x + \sin(\omega_{rf} t + \phi) I_y\right]$$

$$|\psi\rangle^{rot} = \exp(-i\omega_{rf} t I_z)|\psi\rangle$$

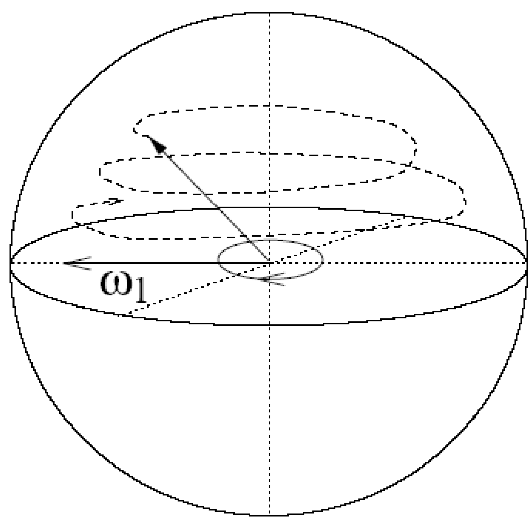
$$\mathcal{H}^{rot} = -\hbar\,(\omega_0 - \omega_{rf})\; I_z - \hbar\omega_1 \left[\cos\phi\, I_x + \sin\phi\, I_y\right]$$

rotating wave approximation

typical strength I_x, I_y : up to 100 kHz



Rotating frame



Lab frame

Nuclear spin Hamiltonian

Coupled spins

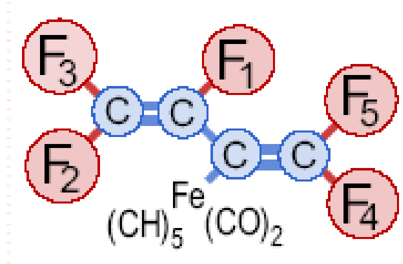
J>0: antiferro mag.

J<0: ferro-mag.

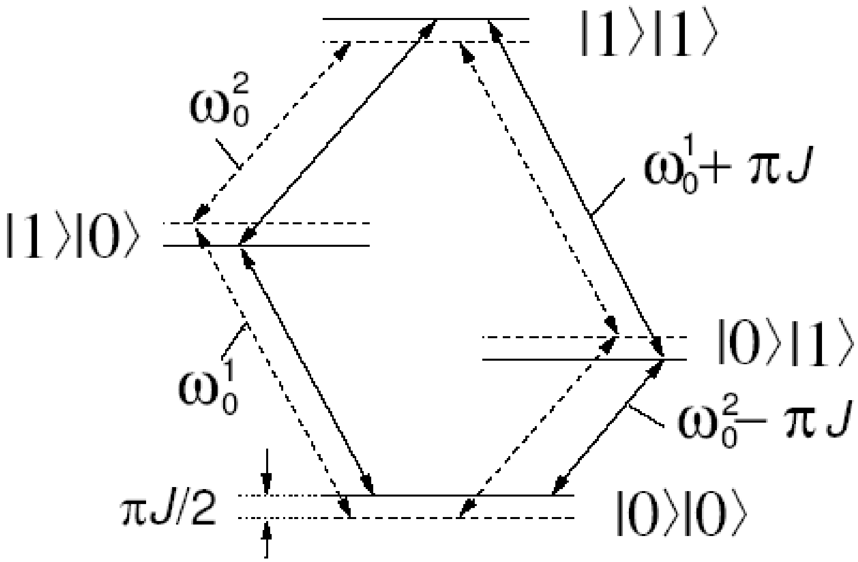
coupling term

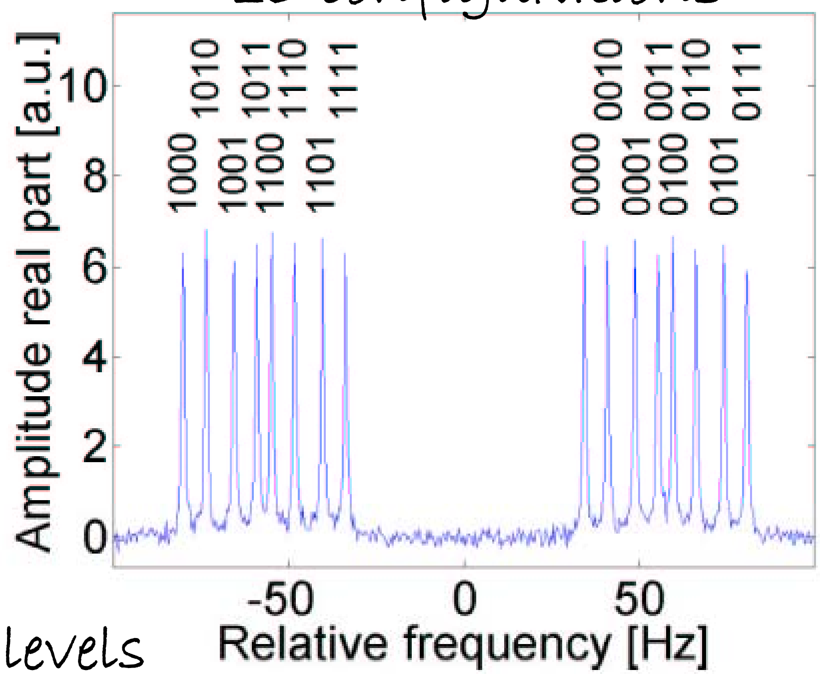
$$\mathcal{H}_J = \hbar \sum_{i<j}^{n} 2\pi J_{ij} I_z^i I_z^j$$

Typical values: *J* up to few 100 Hz

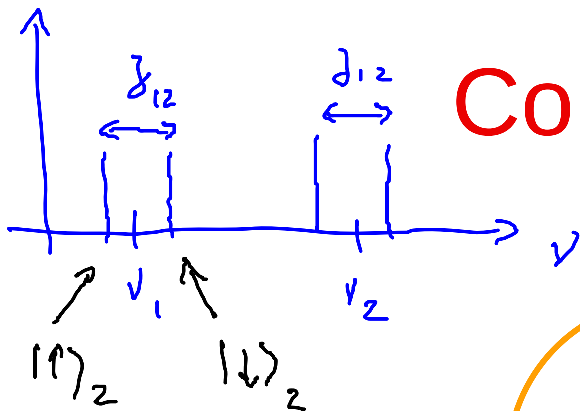


16 configurations



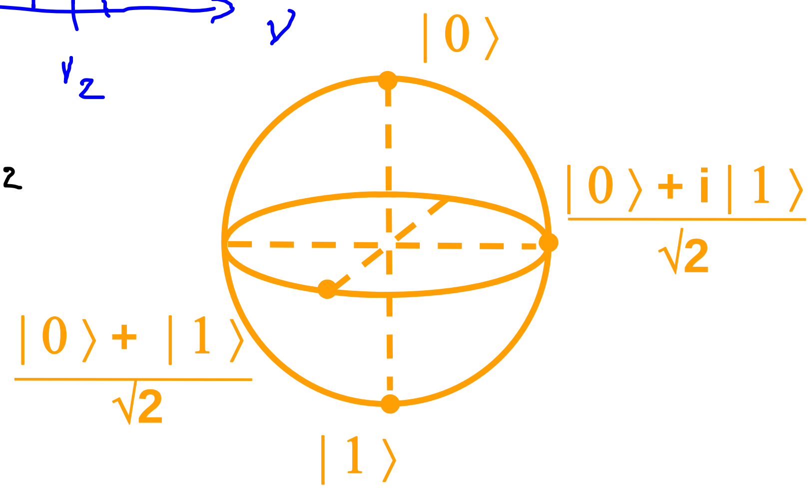


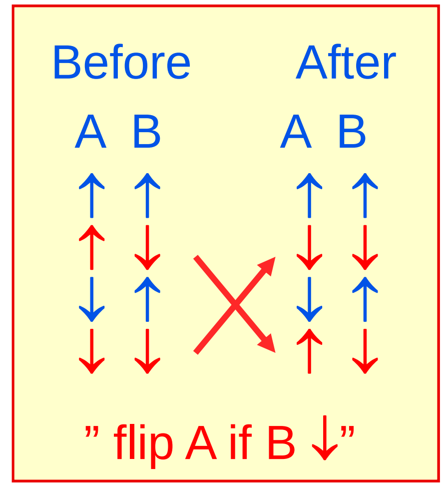
solid (dashed) lines are (un)coupled levels



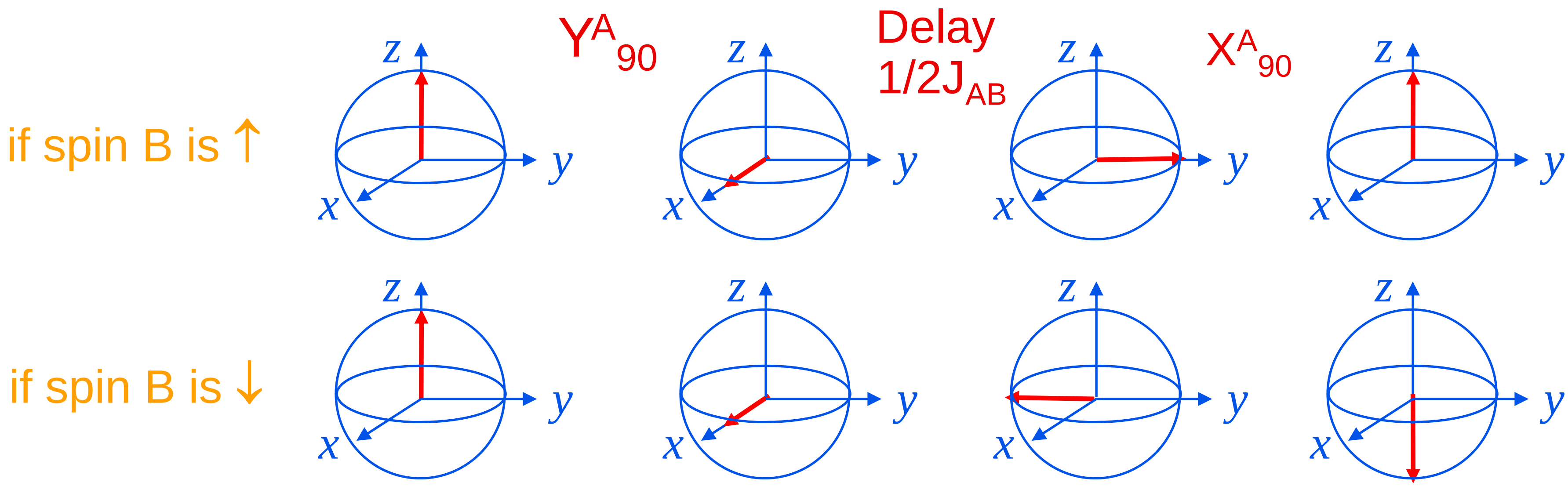
Controlled-NOT in NMR

A target bit
B control bit





wait

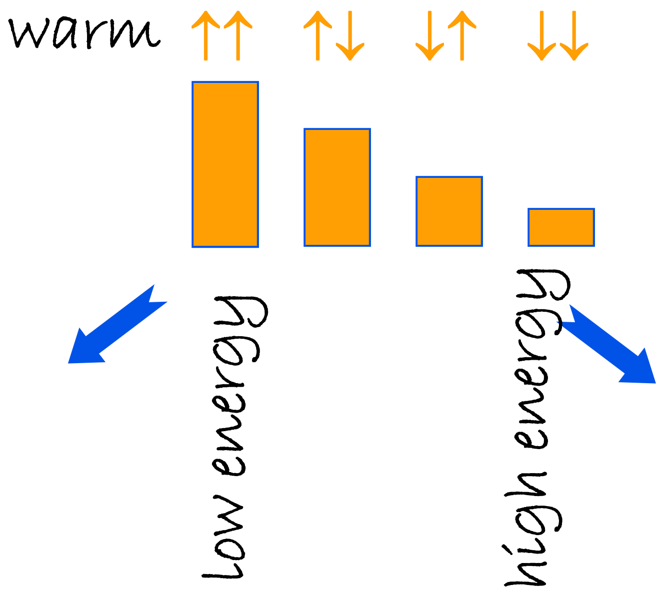


different rotation direction depending on control bit

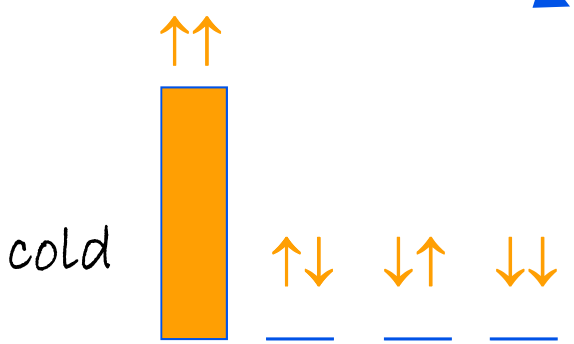
→ time

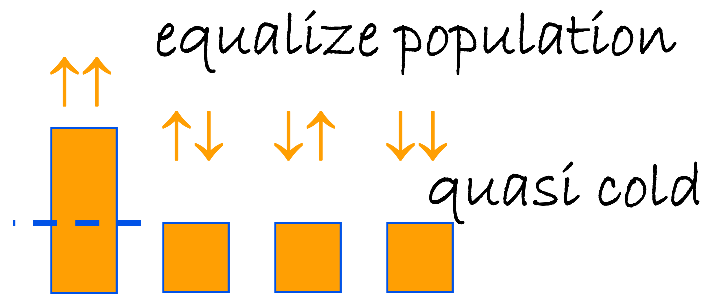
Making room temperature spins look cold

- (Cool to mK)
- Optical pumping
- DNP, …

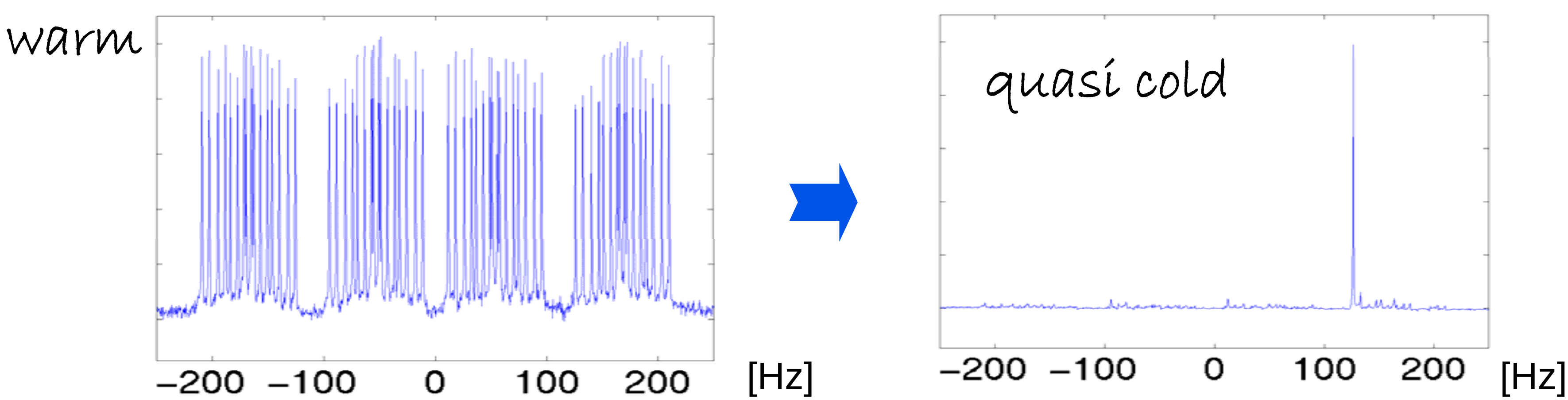


Effective pure state
(Gershenfeld&Chuang, Science ‘97, Cory, Havel & Fahmi, PNAS ‘97)



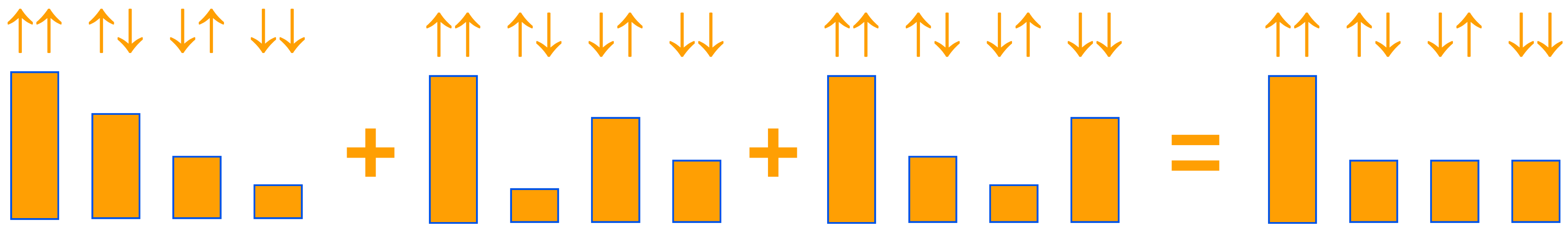


Look exactly like cold spins !



Effective pure state preparation

(1) Add up 2^N-1 experiments (Knill,Chuang,Laflamme, PRA 1998)



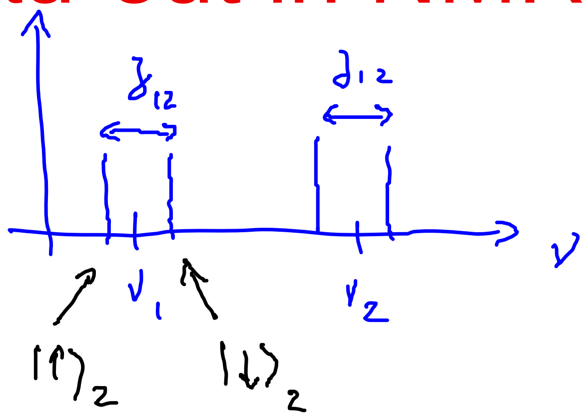
Later ≈ (2^N - 1) / N experiments (Vandersypen *et al.*, PRL 2000)

prepare equal population (on average) and look at deviations from equilibrium.

(2) Work in subspace (Gershenfeld&Chuang, Science 1997)

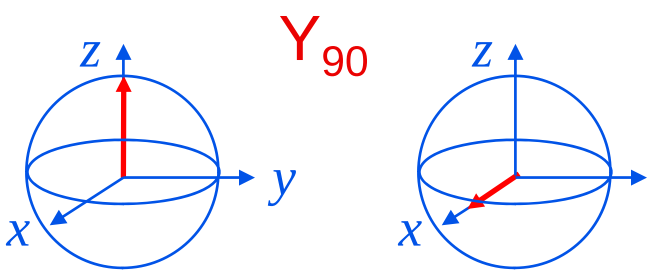
compute with qubit states that have the same energy and thus the same population.

Read-out in NMR



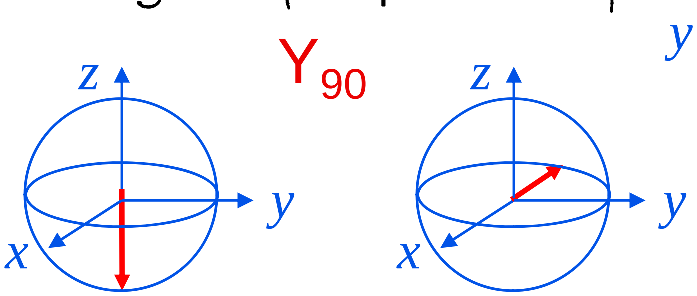
Phase sensitive detection

|0⟩

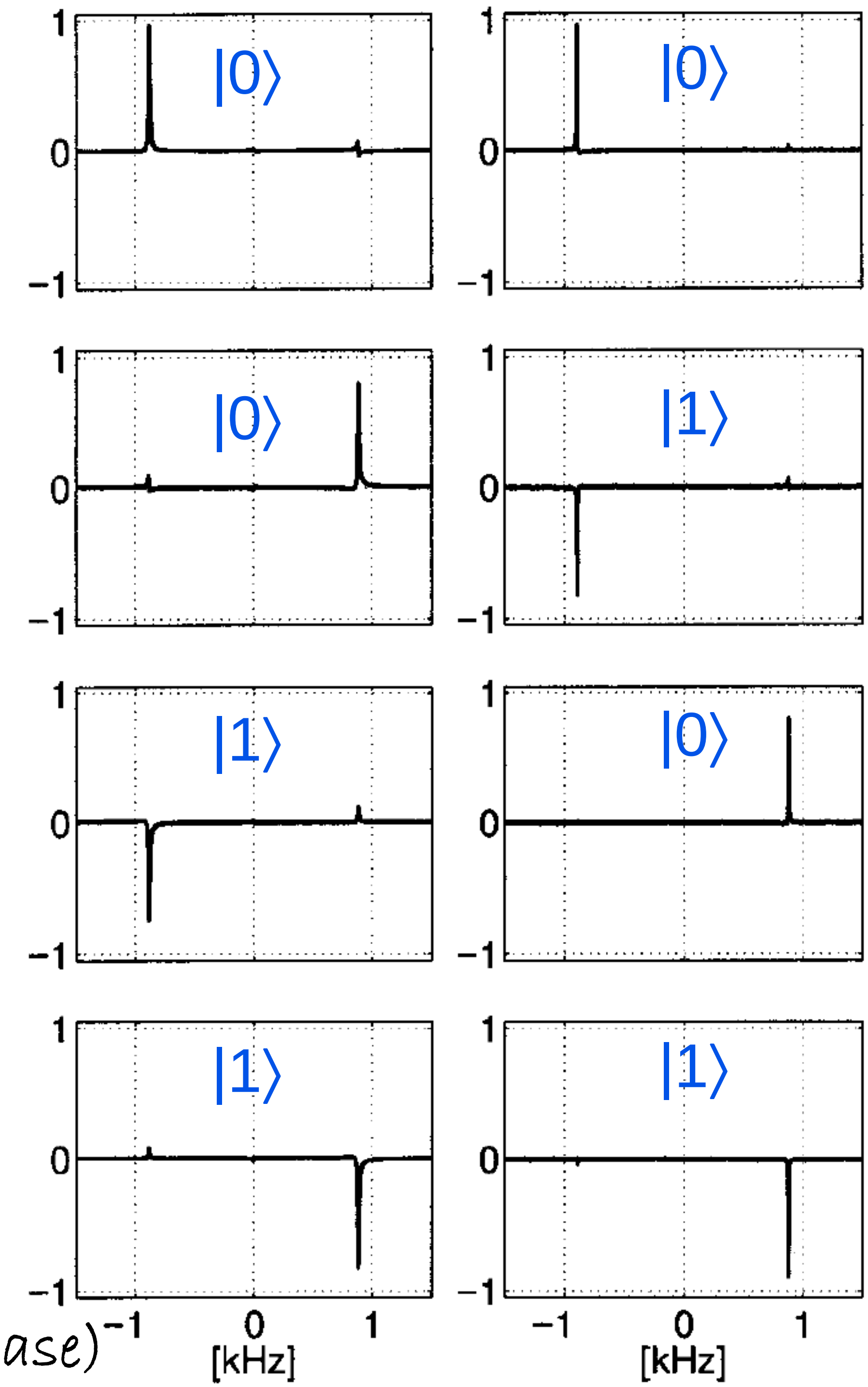


positive signal for |0> (in phase)

|1⟩



negative signal for |1> (out of phase)



Measurements of single systems versus ensemble measurements

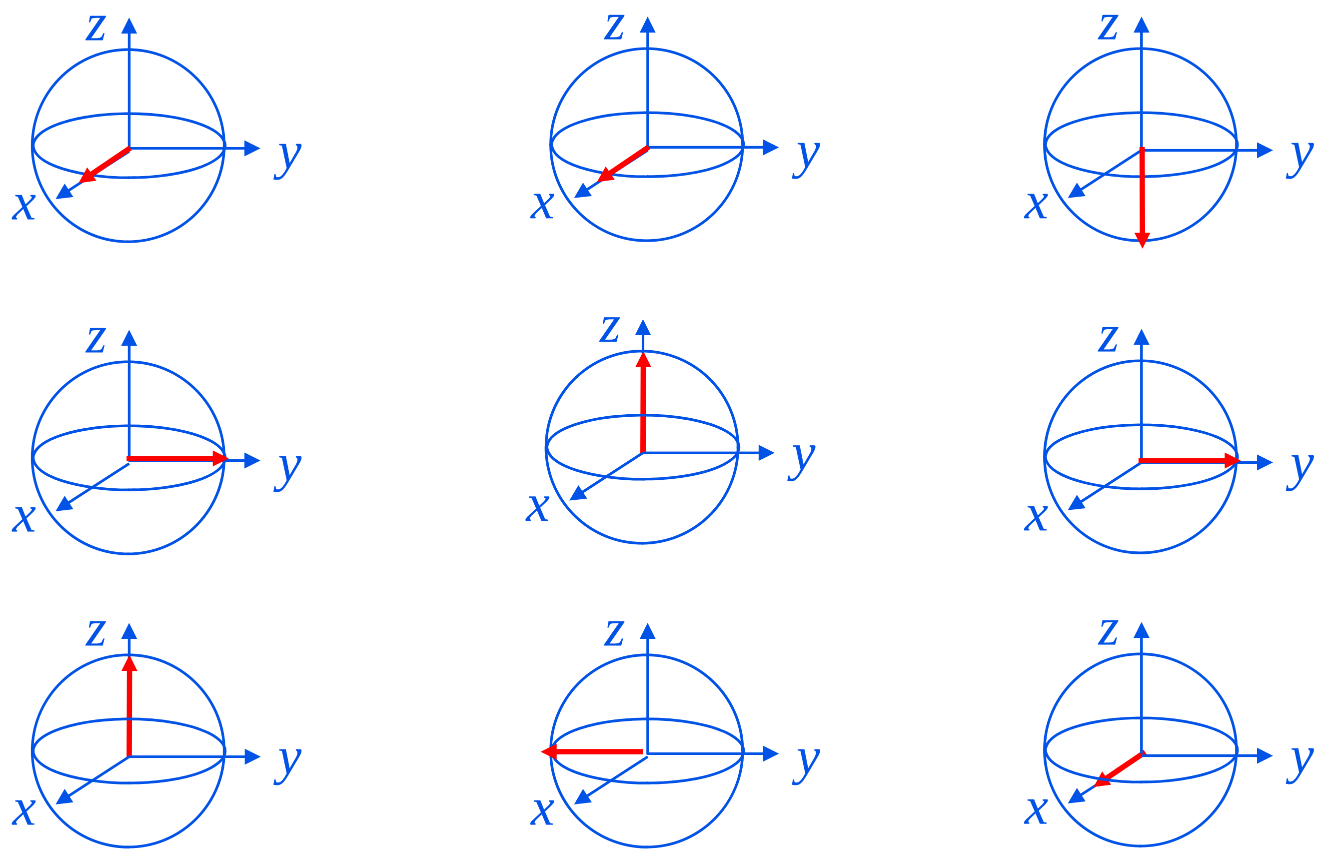
quantum state	$\|00\rangle$	$\|00\rangle + \|11\rangle$	
single-shot bitwise	$\|0\rangle$ and $\|0\rangle$	each bit $\|0\rangle$ *or* $\|1\rangle$	
single-shot "word"wise	$\|00\rangle$	$\|00\rangle$ *or* $\|11\rangle$	**QC**
bitwise average	$\|0\rangle$ and $\|0\rangle$	each bit average of $\|0\rangle$ and $\|1\rangle$	**NMR**
"word"wise average	$\|00\rangle$	average of $\|00\rangle$ and $\|11\rangle$	

adapt algorithms if use ensemble

Quantum state tomography

Look at qubits from different angles

no pulse | after X_{90} | after Y_{90}



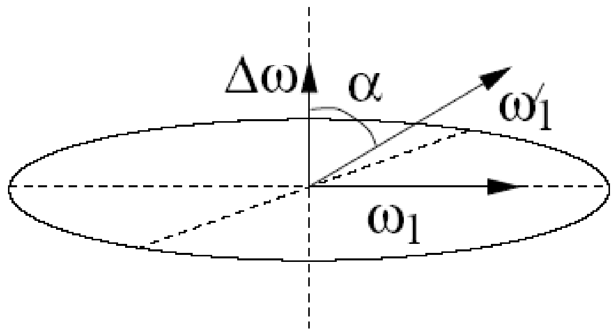
Outline

Survey of NMR quantum computing

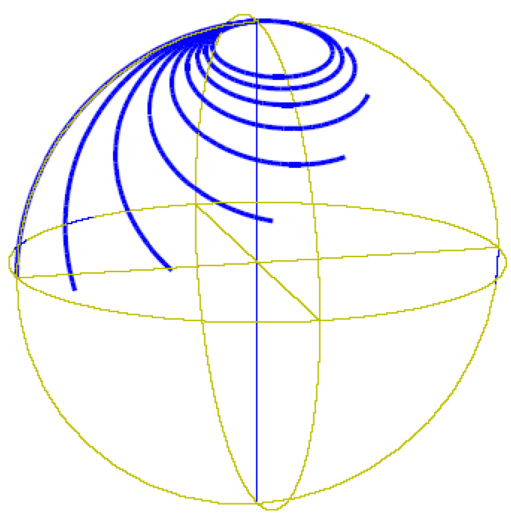
- Principles of NMR QC
- ➡ Techniques for qubit control
- Example: factoring 15
- State of the art
- Outlook

Off-resonance pulses and spin-selectivity

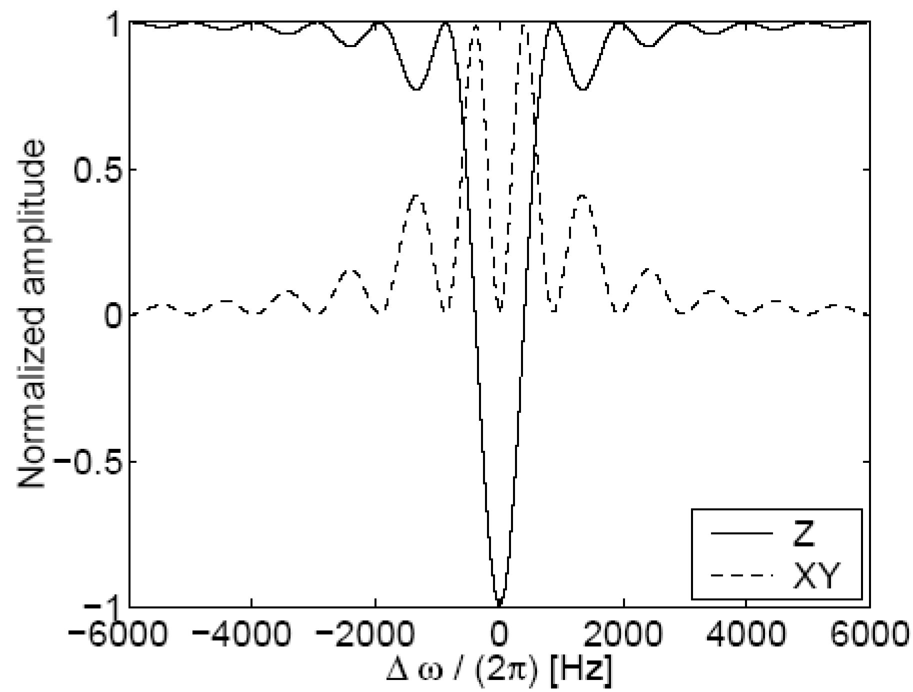
$$\mathcal{H}^{rot} = -\hbar\,(\omega_0 - \omega_{rf})\ I_z - \hbar\omega_1 \left[\cos\phi\, I_x + \sin\phi\, I_y\right]$$



off-resonant pulses induce eff. σ_z rotation in addition to $\sigma_{x,y}$



spectral content of a square pulse

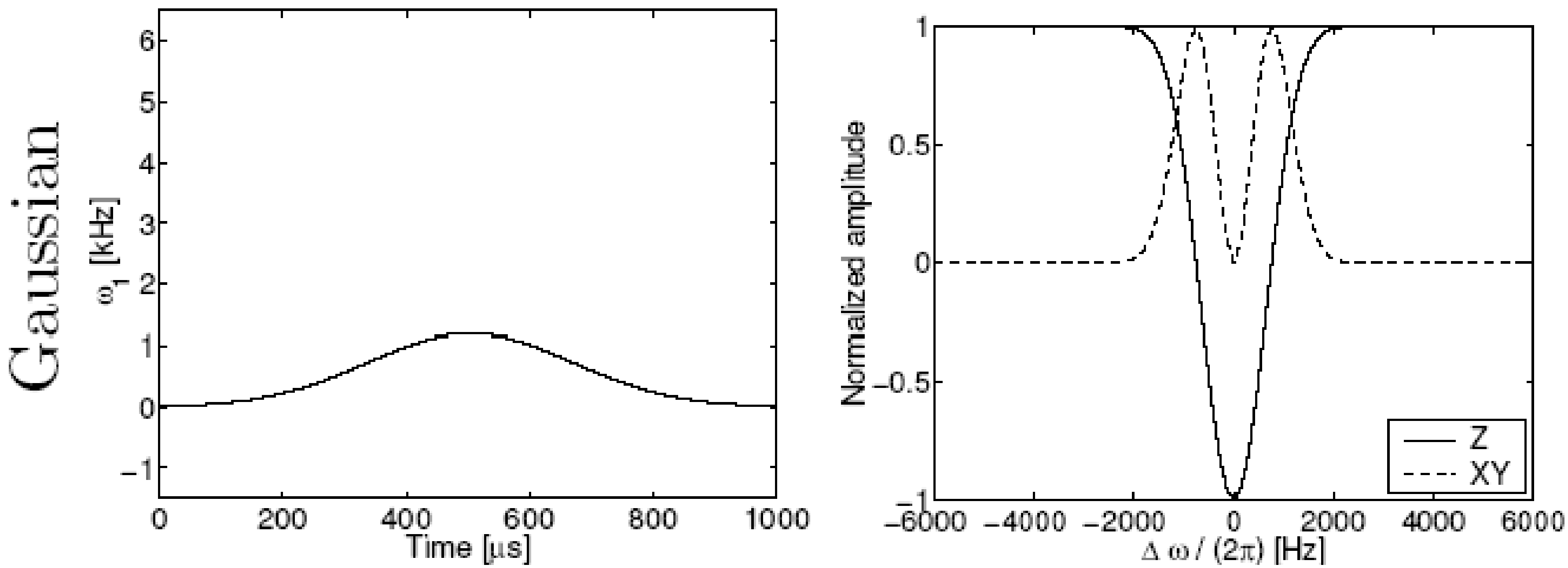


may induce transitions in other qubits

Pulse shaping for improved spin-selectivity

gaussian pulse profile

gaussian spectrum



less cross-talk

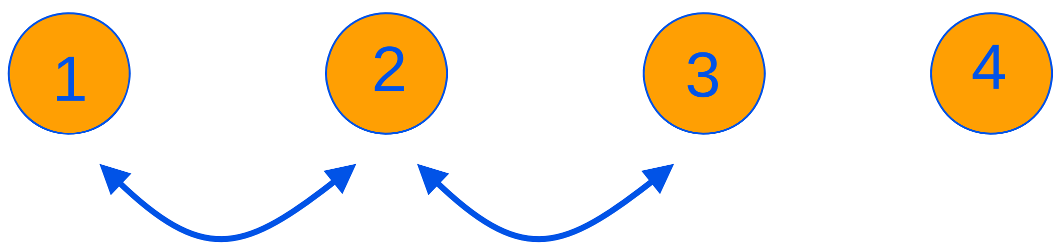
Missing coupling terms: Swap

How to couple distant qubits with only nearest neighbor physical couplings?

Missing couplings: swap states along qubit network

$$SWAP_{12} = CNOT_{12}\ CNOT_{21}\ CNOT_{12}$$

as discussed in exercise class

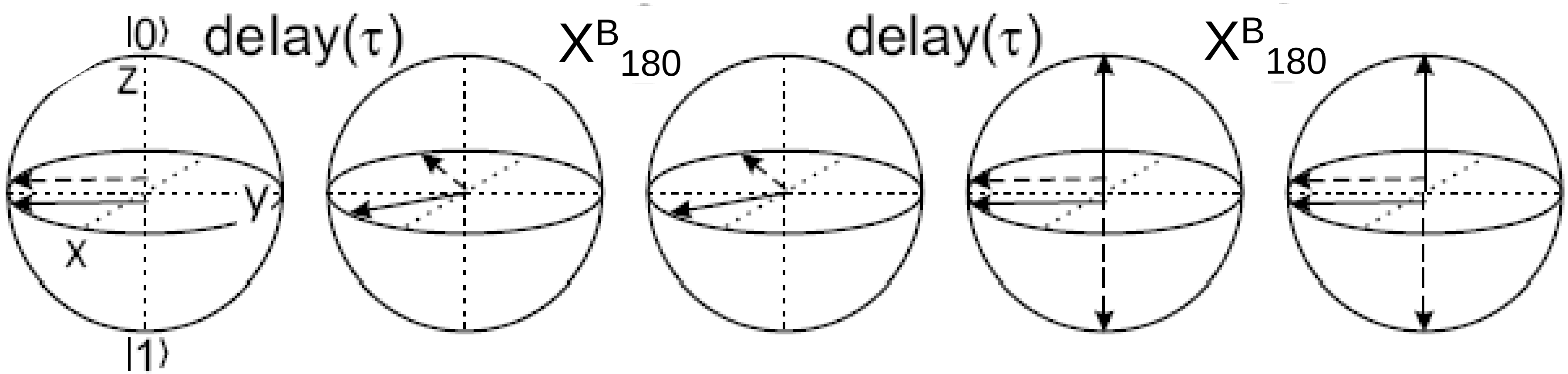


"only" a linear overhead ...

Undesired couplings: refocus

remove effect of coupling *during delay times*

opt. 1: act on qubit B



opt. 2: act on qubit A

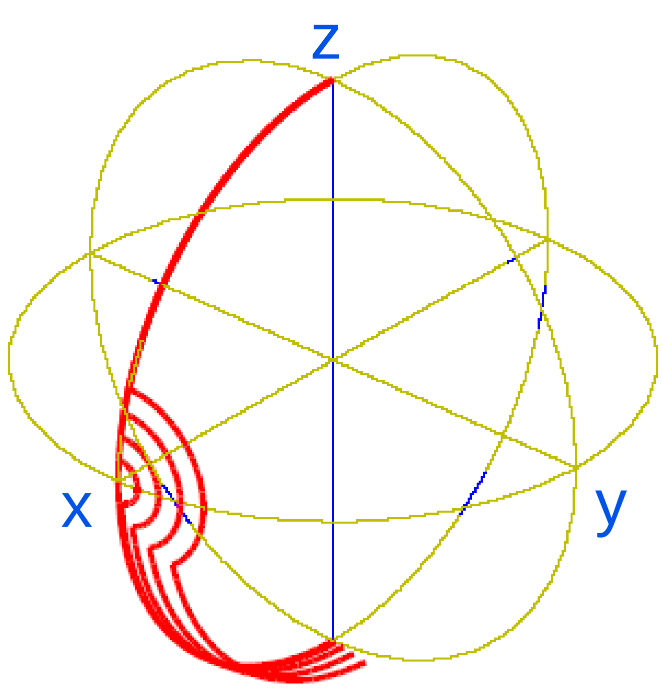
- There exist efficient extensions for arbitrary coupling networks
- Refocusing can also be used to remove unwanted Zeeman terms

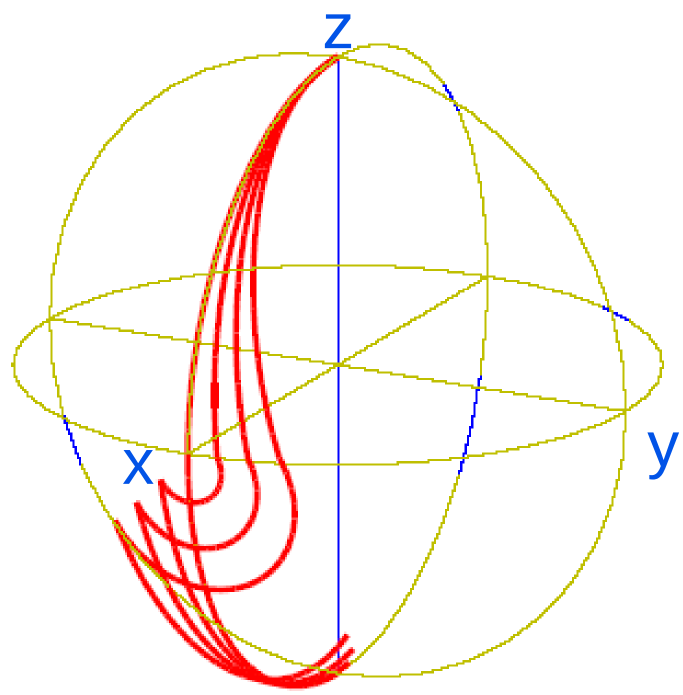
Composite pulses

Example: $Y_{90}X_{180}Y_{90}$

corrects for
under/over-rotation

corrects for
off-resonance





However: doesn’t work for arbitrary input state
But: there exist composite pulses that work for all input states

Molecule selection

A quantum computer is a *known* molecule.
Its desired properties are:

- spins 1/2 (^{1}H, ^{13}C, ^{19}F, ^{15}N, ...)
- long T_1's and T_2's
- heteronuclear, or large chemical shifts
- good J-coupling network (clock-speed)

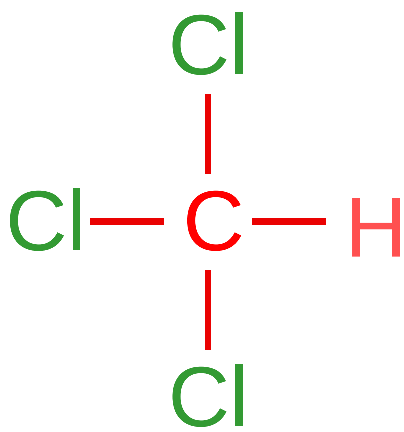
- stable, available, soluble, ...

required to make spins of same type addressable

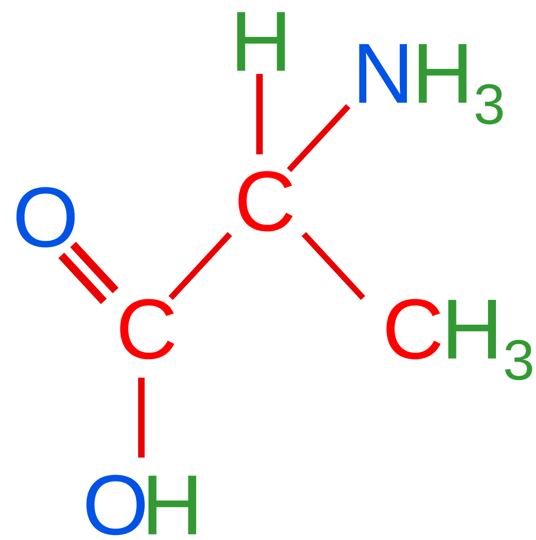
Quantum computer molecules (1)

red nuclei are used
as qubits:

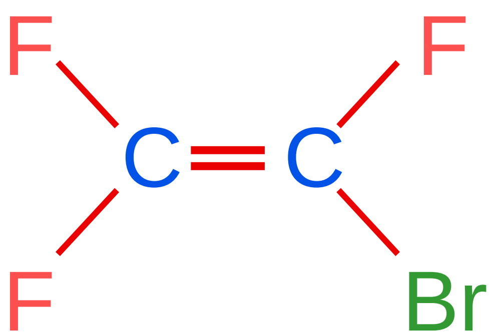
Grover / Deutsch-Jozsa



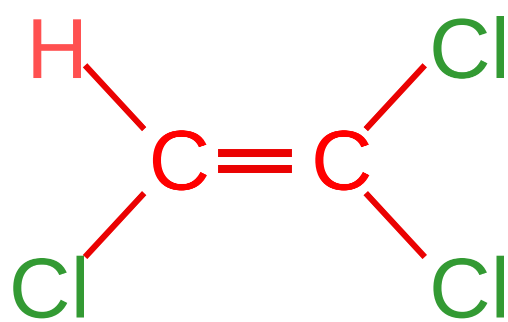
Q. Error correction



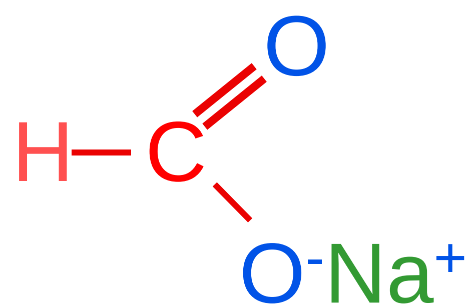
Logical labeling / Grover



Teleportation

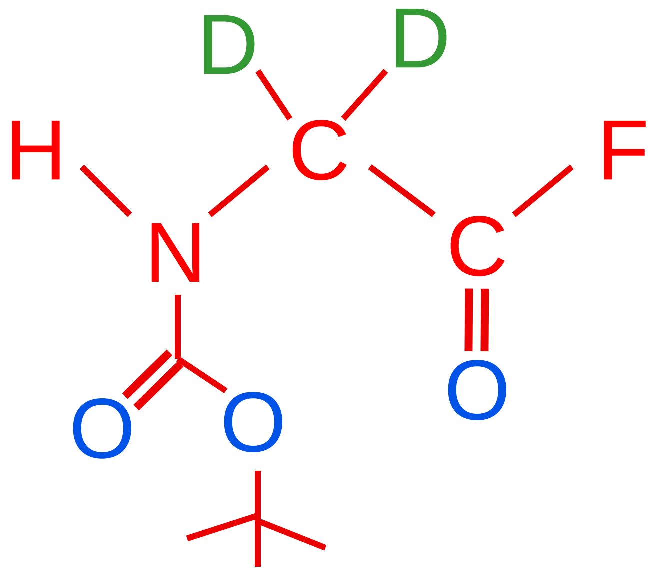


Q. Error Detection

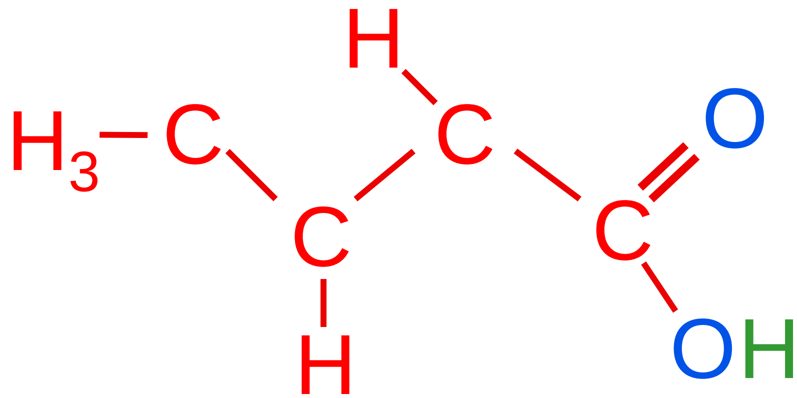


Quantum computer molecules (2)

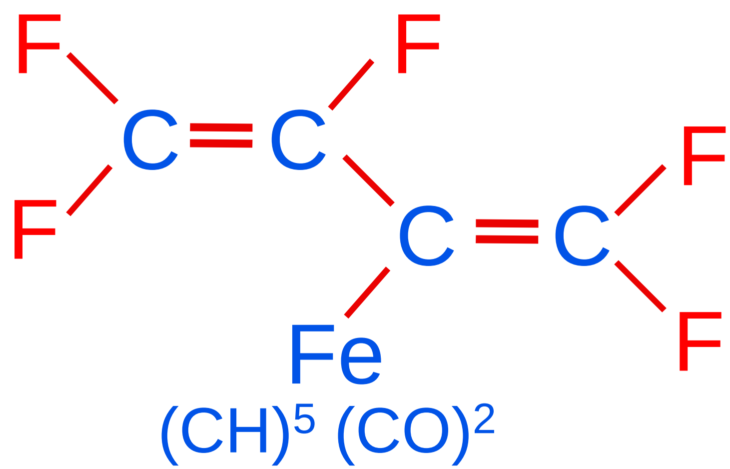
Deutsch-Jozsa



7-spin coherence



Order-finding



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The good news

- Quantum computations have been demonstrated in the lab
- A high degree of control was reached, permitting hundreds of operations in sequence
- A variety of tools were developed for accurate unitary control over multiple coupled qubits
  - ⇨ *useful in other quantum computer realizations*
- Spins are natural, attractive qubits

Scaling

We do not know how to scale liquid NMR QC

Main obstacles:

- Signal after initialization ~ 1 / 2^{n} [at least in practice]
- Coherence time typically goes down with molecule size
- We have not yet reached the accuracy threshold ...

Main sources of errors in NMR QC

Early on (heteronuclear molecules)

inhomogeneity RF field

Later (homonuclear molecules)

*J c*oupling during RF pulses

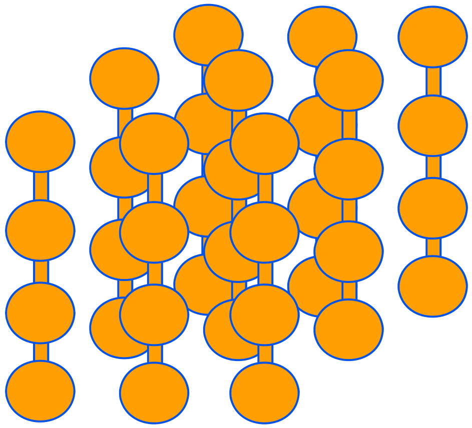
Finally

decoherence

Solid-state NMR ?

molecules in
solid matrix

Cory et al

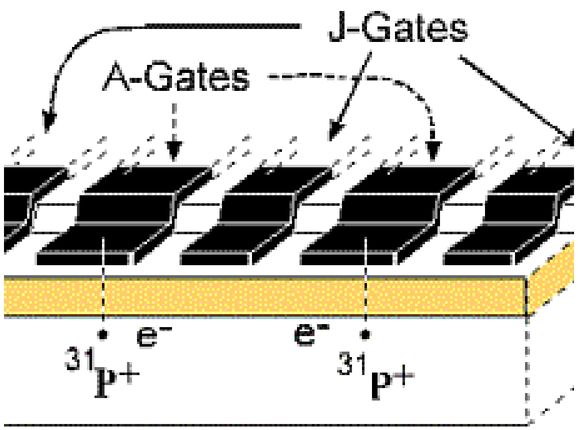


Yamaguchi & Yamamoto, 2000

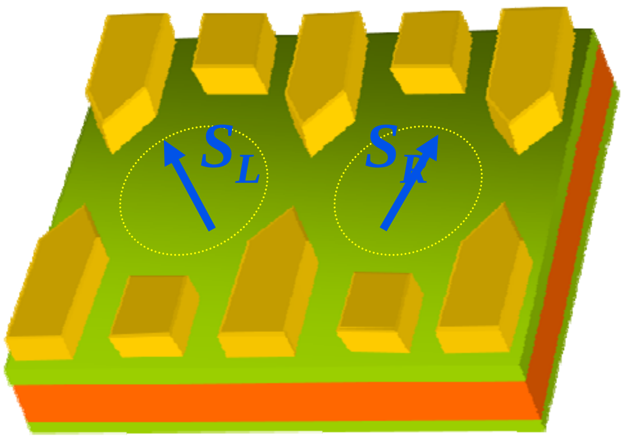
$$\mathcal{H}_J = \hbar \sum_{i<j} 2\pi J_{ij} \vec{I}^i \cdot \vec{I}^j = \hbar \sum_{i<j} 2\pi J_{ij} (I_x^i I_x^j + I_y^i I_y^j + I_z^i I_z^j)$$

$$\mathcal{H}_D = \sum_{i<j} \frac{\mu_0 \gamma_i \gamma_j \hbar}{4\pi |\vec{r}_{ij}|^3} \left[\vec{I}^i \cdot \vec{I}^j - \frac{3}{|\vec{r}_{ij}|^2} (\vec{I}^i \cdot \vec{r}_{ij})(\vec{I}^j \cdot \vec{r}_{ij}) \right]$$

Electron spin qubits



Kane, Nature 1998



Loss & DiVincenzo, PRA 1998

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Quantum Factoring

Find the prime factors of N: chose a and find order r.

$$f(x) = a^x \bmod N$$

a: coprime with N

N: composite number

Results from number theory:

- f is periodic in x (period r)
- $\gcd(a^{r/2} \pm 1, N)$ is a factor of N

Quantum factoring: find r

Complexity of factoring numbers of length L:

Quantum: $\sim L^3$ P. Shor (1994)

Classically: $\sim e^{L/3}$

Widely used crypto systems (RSA) would become insecure.

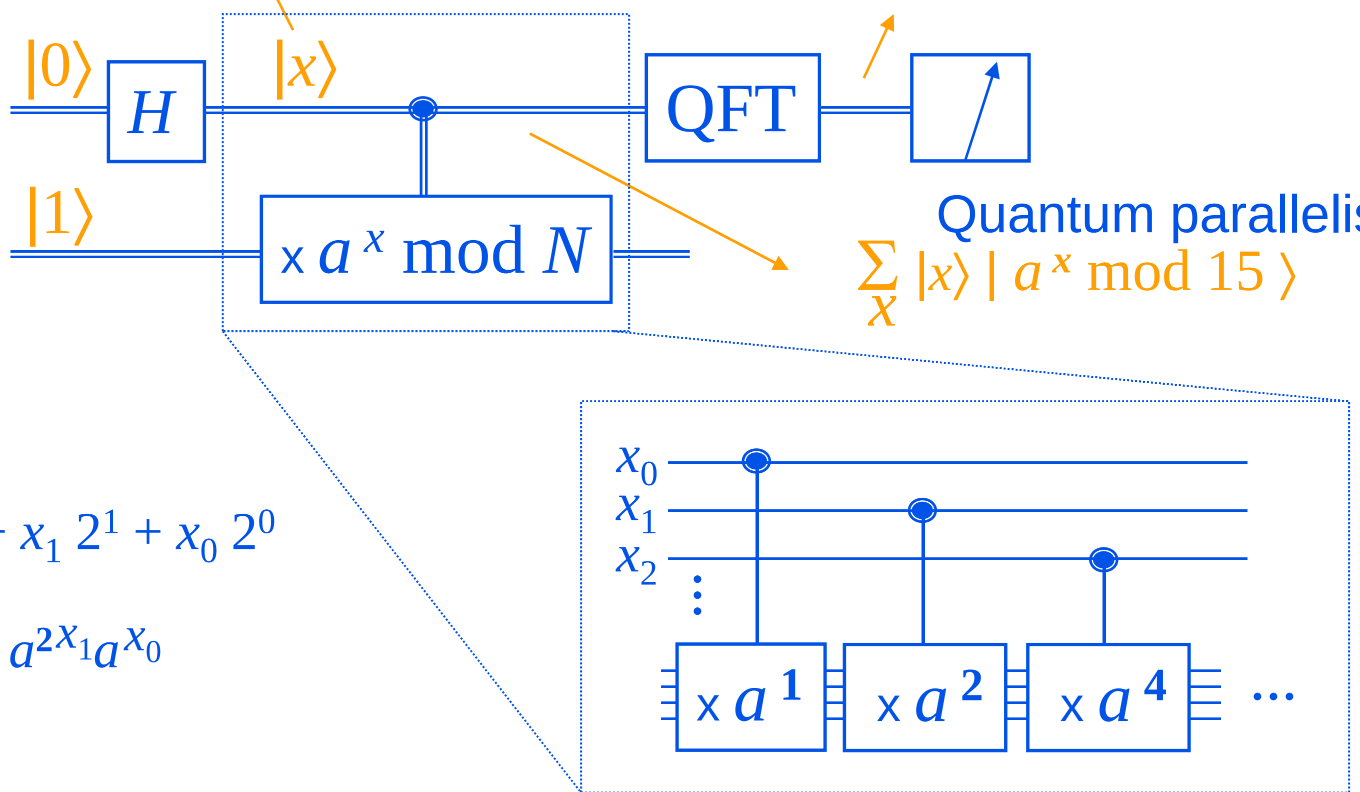
Factoring 15 - schematic

$|x\rangle = |0\rangle + |1\rangle + \ldots + |2^{2L}\text{-}1\rangle$

$\sum_k |k2L/r\rangle$ Interference

2 L bits
3 qubits

$L = \log_2(15)$
4 qubits



$x = \ldots + x_2\, 2^2 + x_1\, 2^1 + x_0\, 2^0$

$a^{x} = \ldots\, a^{4x_2}\, a^{2x_1} a^{x_0}$

a = 4, 11 $\Rightarrow$ a^2 mod 15 = 1 $\Rightarrow$ "easy" case period 2

a = 2, 7, 8, 13 $\Rightarrow$ a^4 mod 15 = 1 $\Rightarrow$ "hard" case period 4

a = 14 $\Rightarrow$ fails

Quantum Fourier transform and the FFT

FFT →

[1 1 1 1 1 1 1 1]	[1 . . . .]
[1 . 1 . 1 . 1 .]	[1 . . . 1 . . .]
[1 . . . 1 . . .]	[1 . 1 . 1 . 1 .]
[1 . . . .]	[1 1 1 1 1 1 1 1]
[1 . . . 1 . . .]	[1 . 1 . 1 . 1 .]
[. 1 . . . 1 . .]	[1 . -i . -1 . i .]
[. . 1 . . . 1 .]	[1 . -1 . 1 . -1 .]
[. . . 1 . . . 1]	[1 . i . -1 . -i .]

The FFT (and QFT)
- Inverts the period
- Removes the off-set

$a = 11$

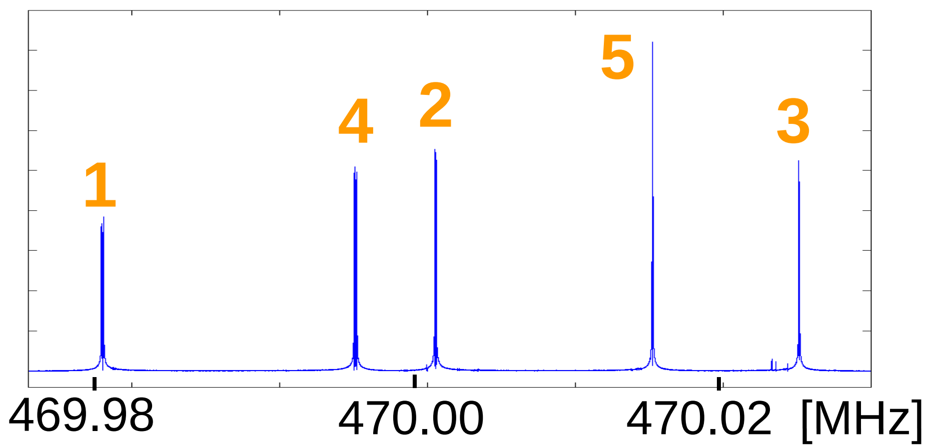
$$|\psi_3\rangle = |0\rangle|0\rangle + |1\rangle|2\rangle + |2\rangle|0\rangle + |3\rangle|2\rangle + |4\rangle|0\rangle + |5\rangle|2\rangle + |6\rangle|0\rangle + |7\rangle|2\rangle$$

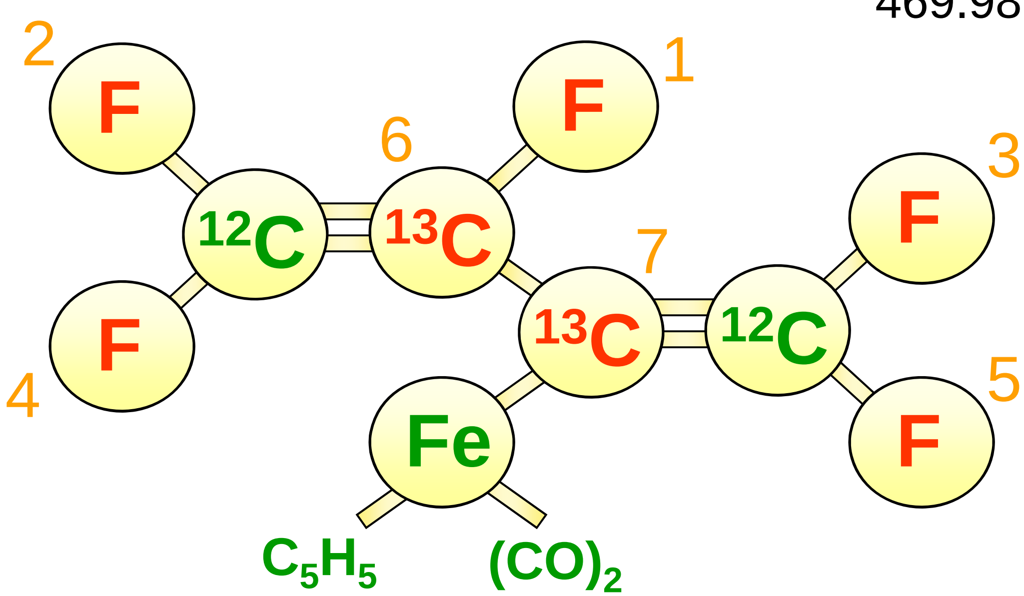
$$= (|0\rangle + |2\rangle + |4\rangle + |6\rangle)|0\rangle + (|1\rangle + |3\rangle + |5\rangle + |7\rangle)|2\rangle$$ after mod exp

$$|\psi_4\rangle = (|0\rangle + |4\rangle)|0\rangle + (|0\rangle - |4\rangle)|2\rangle$$ after QFT

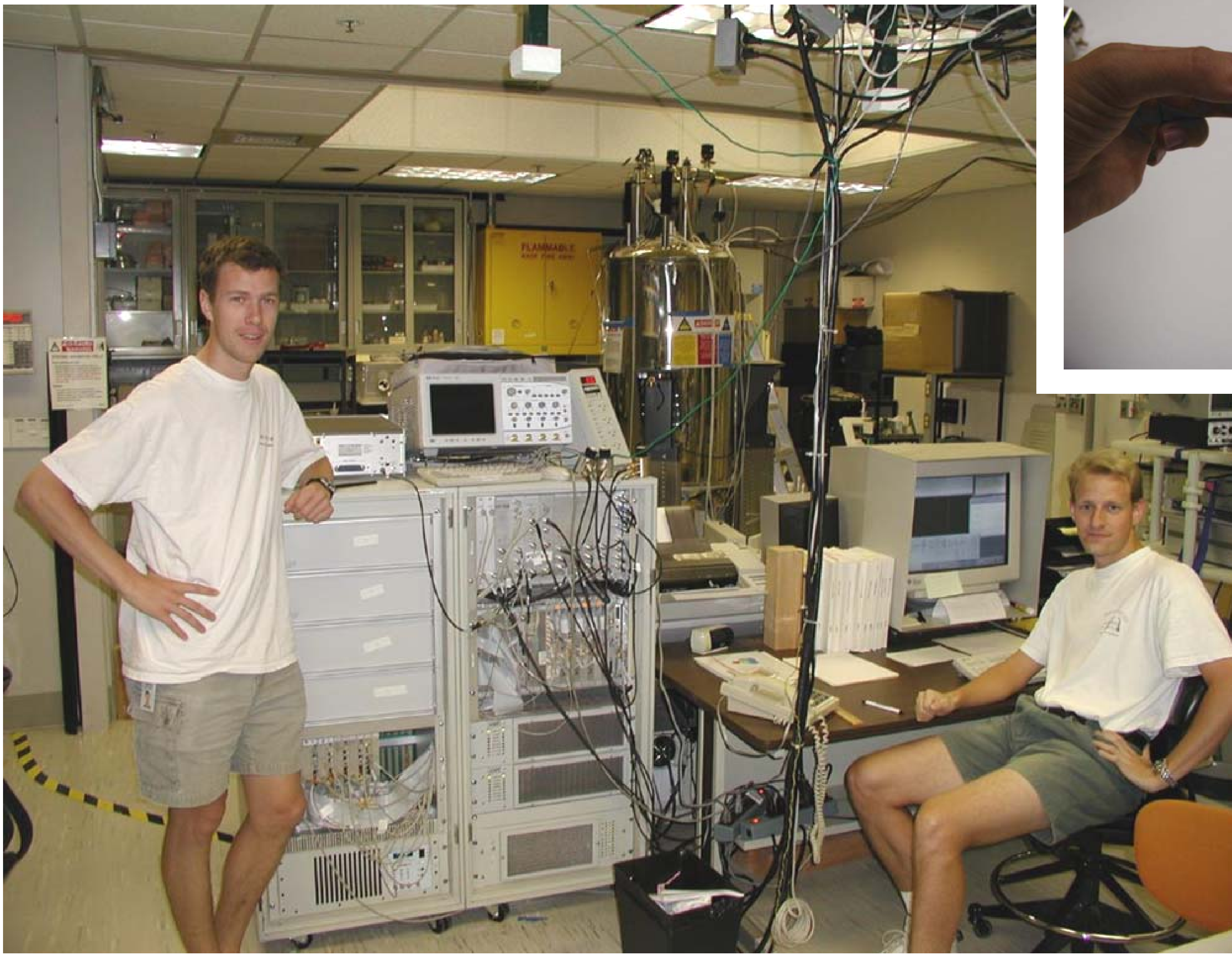
Experimental approach

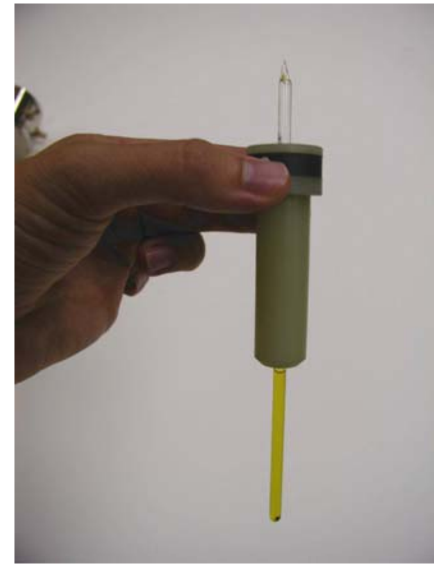
- 11.7 Tesla Oxford superconducting magnet; room temperature bore
- 4-channel Varian spectrometer; need to address and keep track of 7 spins
  - phase ramped pulses
  - software reference frame
- Shaped pulses
- Compensate for cross-talk
- Unwind coupling during pulse





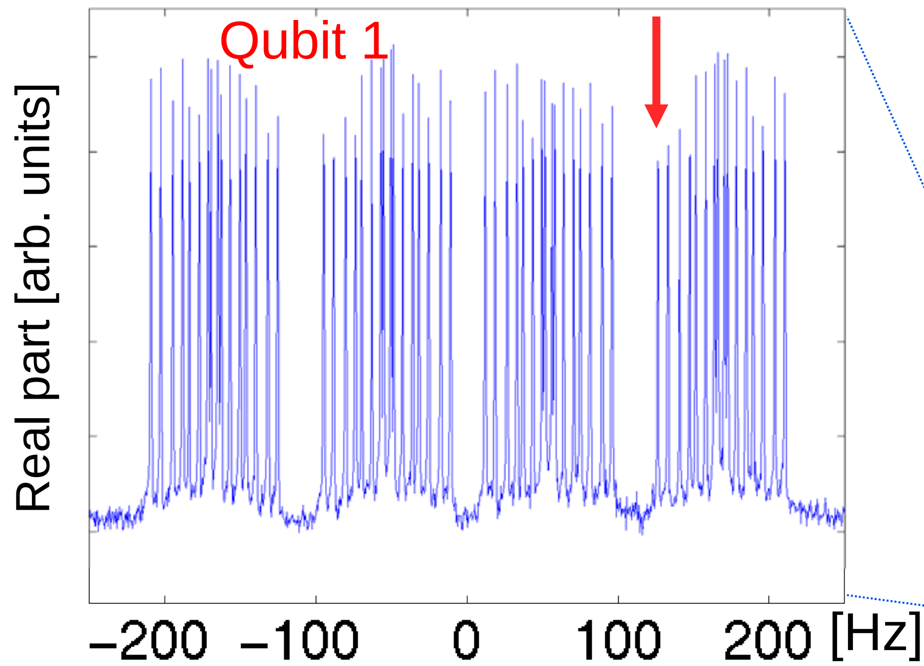
- Larmor frequencies
  - 470 MHz for ^{19}F ~25 mK
  - 125 MHz for ^{13}C
- J - couplings: 2 - 220 Hz
- coherence times: 1.3 - 2 s

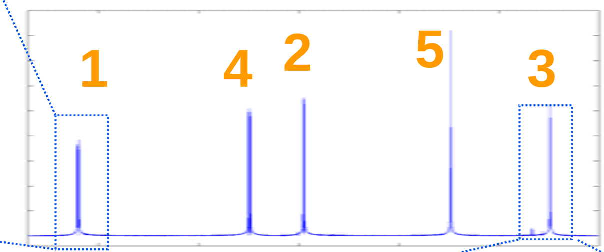

FLAMMABLE

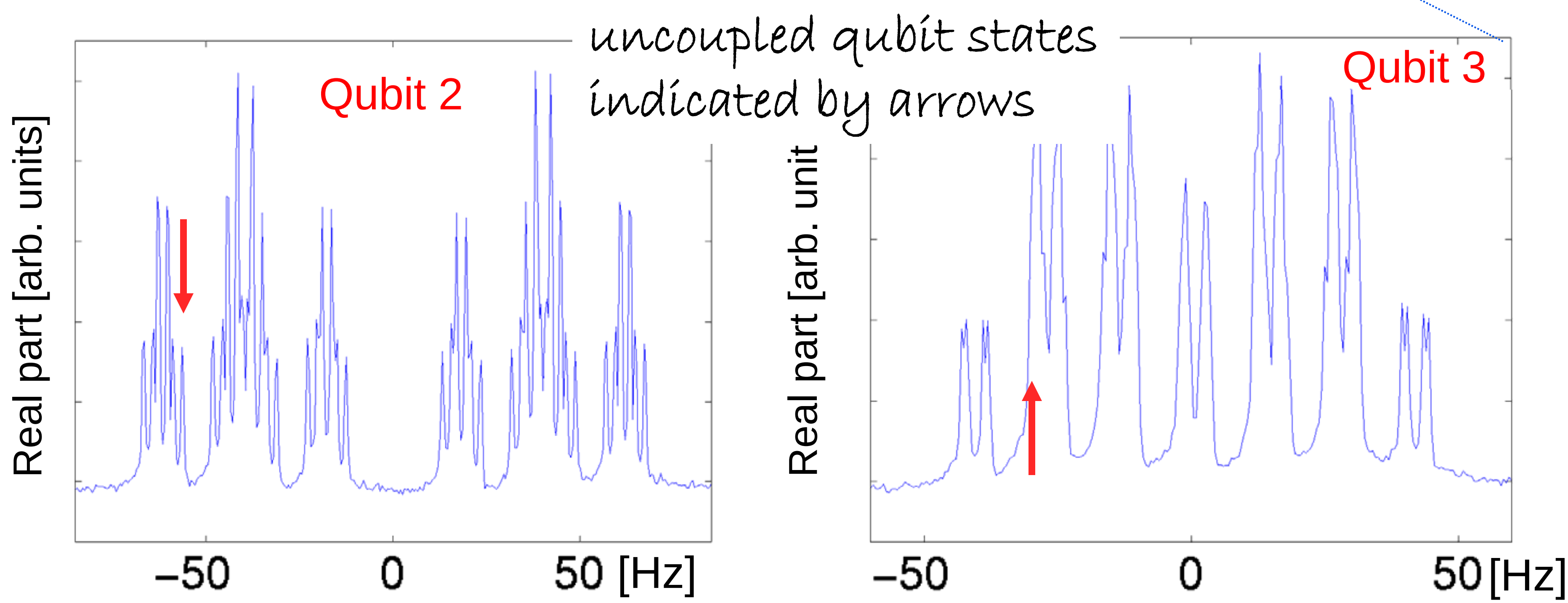


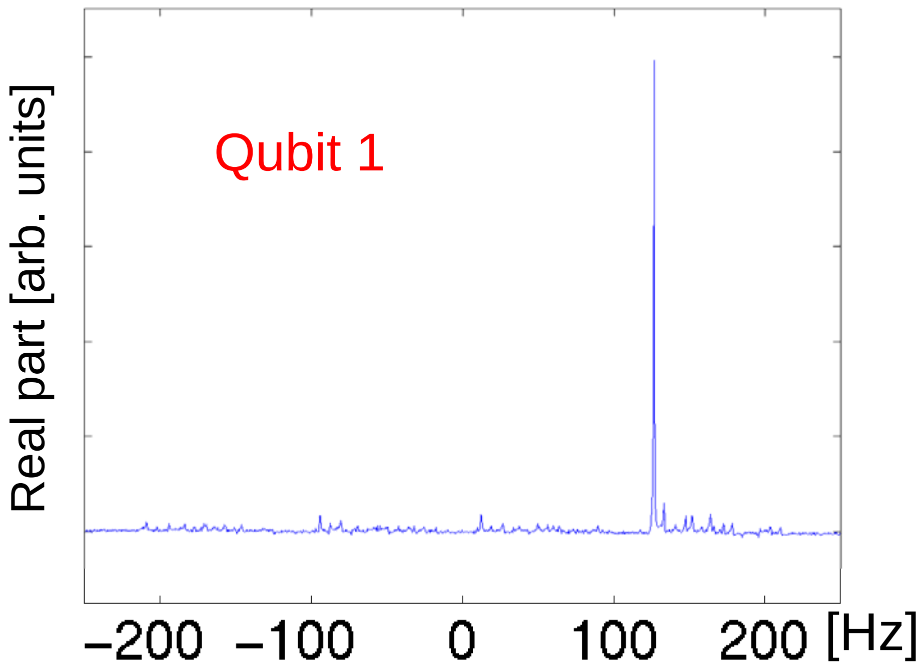
Thermal Equilibrium Spectra

- line splitting due to J-coupling
- all lines present





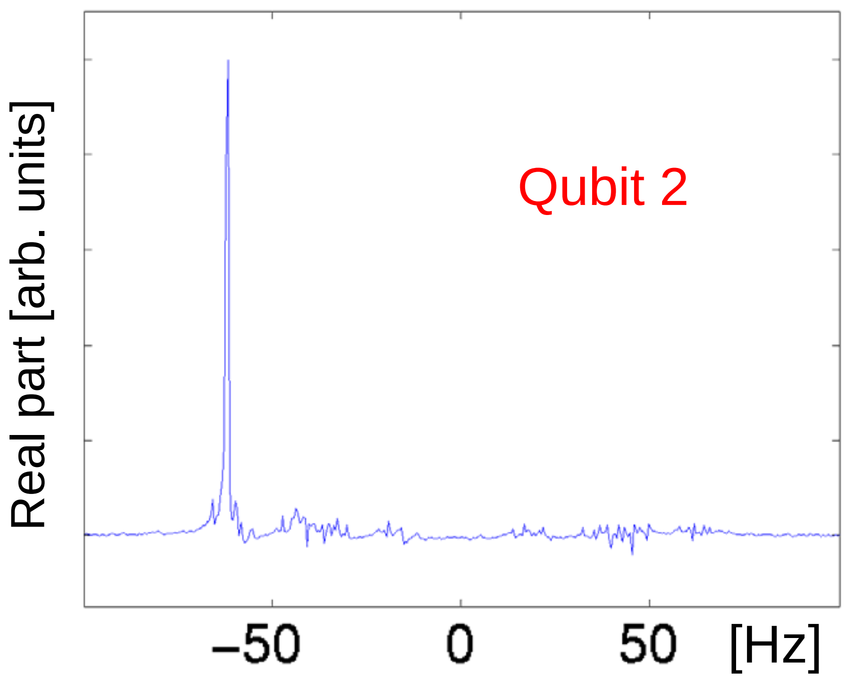


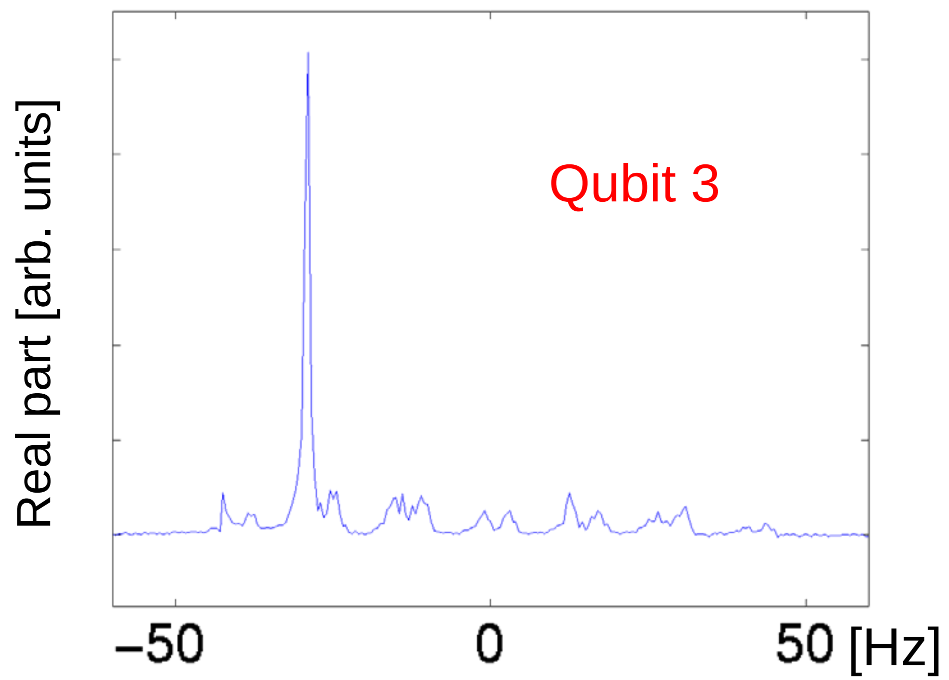


Spectra after state initialization

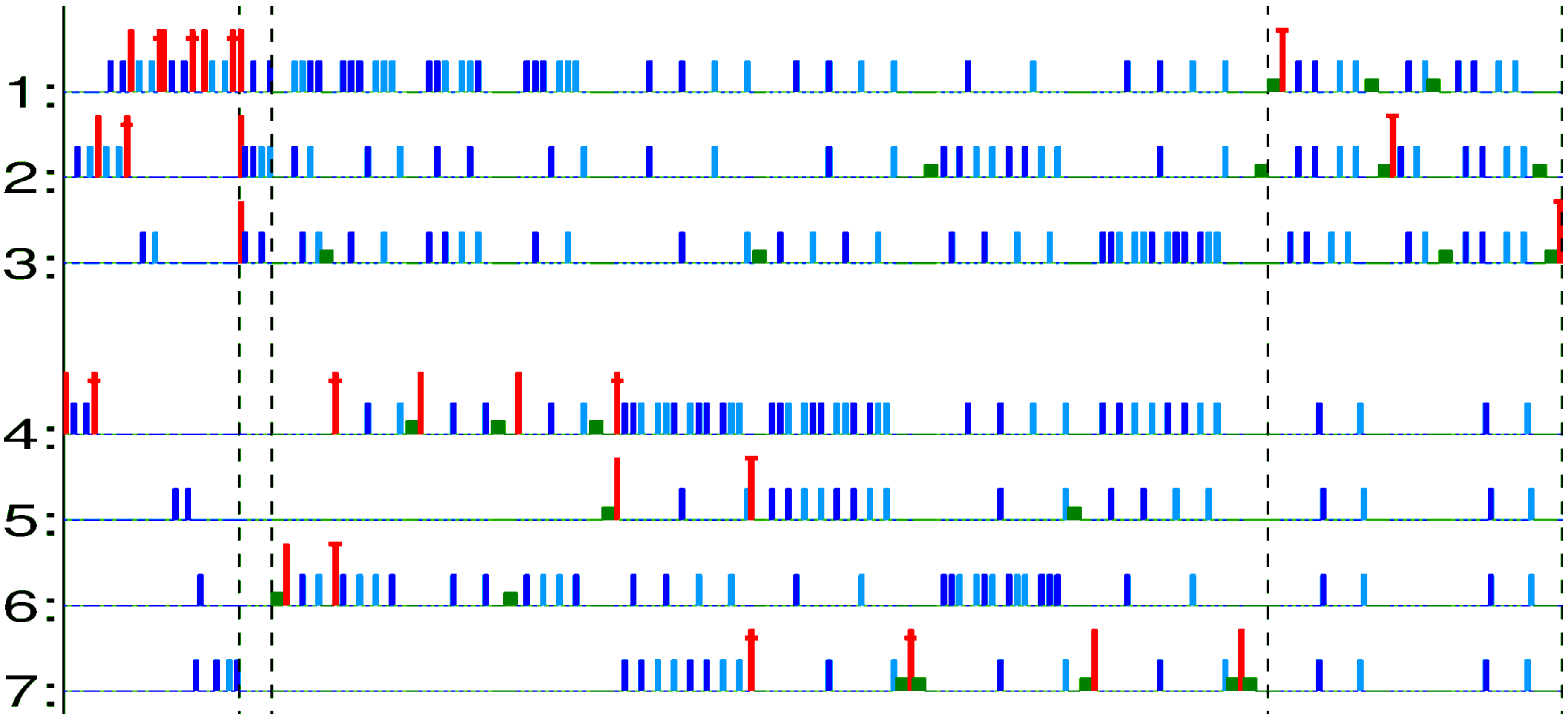
- only the |00 … 0 ⟩ line remains
- the other lines are averaged away by adding up multiple experiments

RT spins appear cold!





Pulse sequence (*a*=7)



π/2 X- or Y-rotations (H and gates)

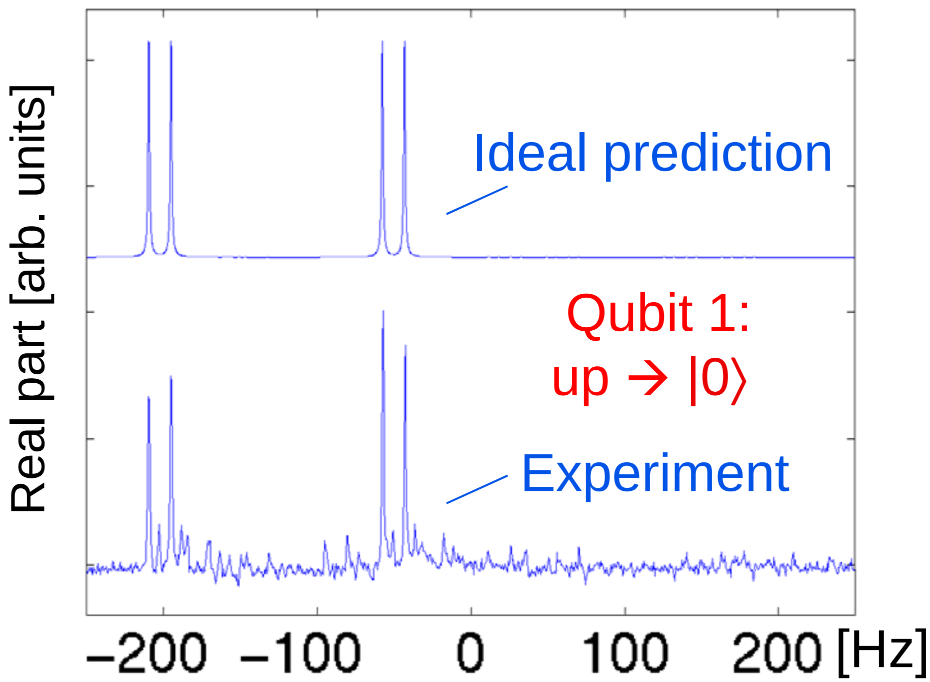
π X-rotations (refocusing)

Z - rotations

> 300 pulses, ≈ 720 ms

“Easy” case (a=11)

period 2



321

$\lvert 000\rangle$	**0**	
$\lvert 100\rangle$	**4**	

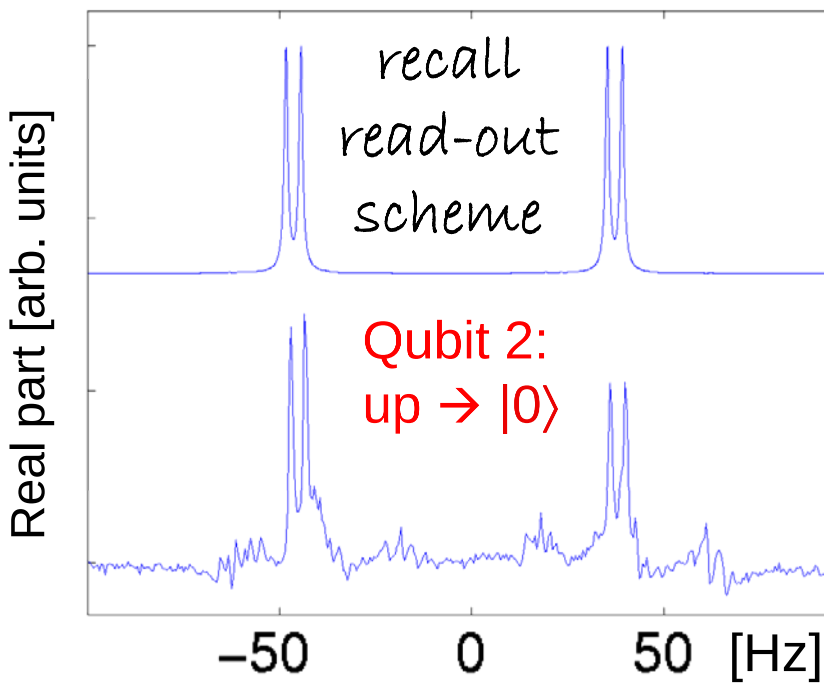
➡ $8 / r = 4$

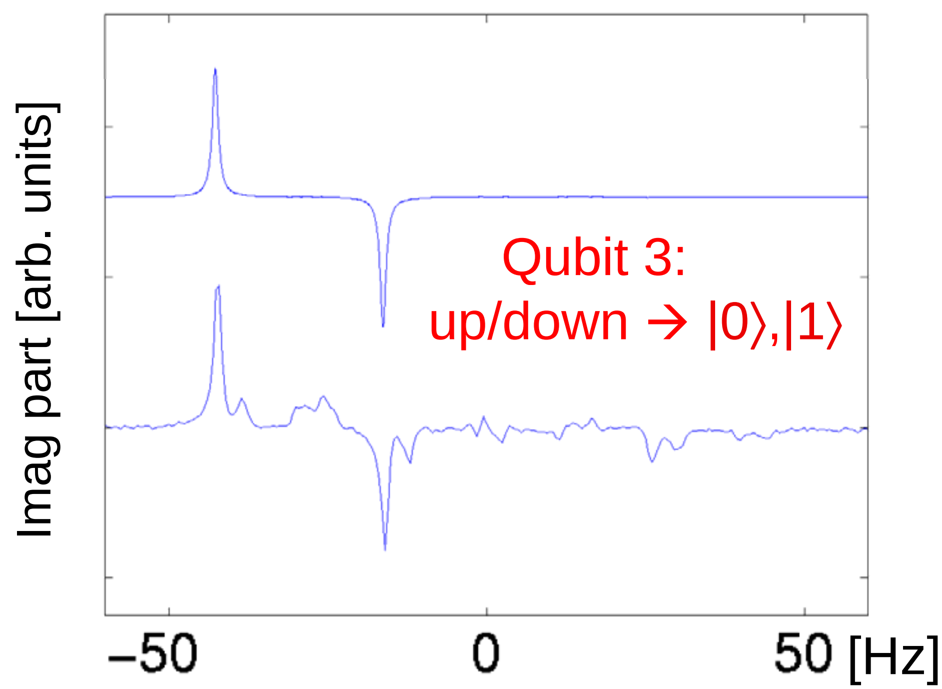
$r = 2$ period

$\gcd(11^{2/2} - 1, 15) = 5$

$\gcd(11^{2/2} + 1, 15) = 3$

15 = 3 x 5





“Hard” case (*a*=7)

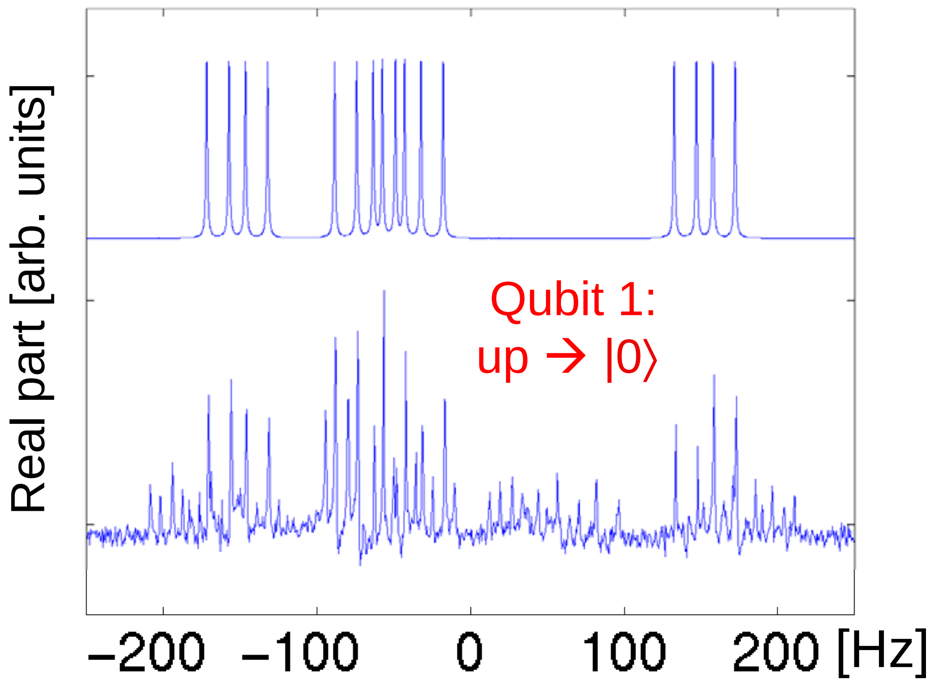
period 4

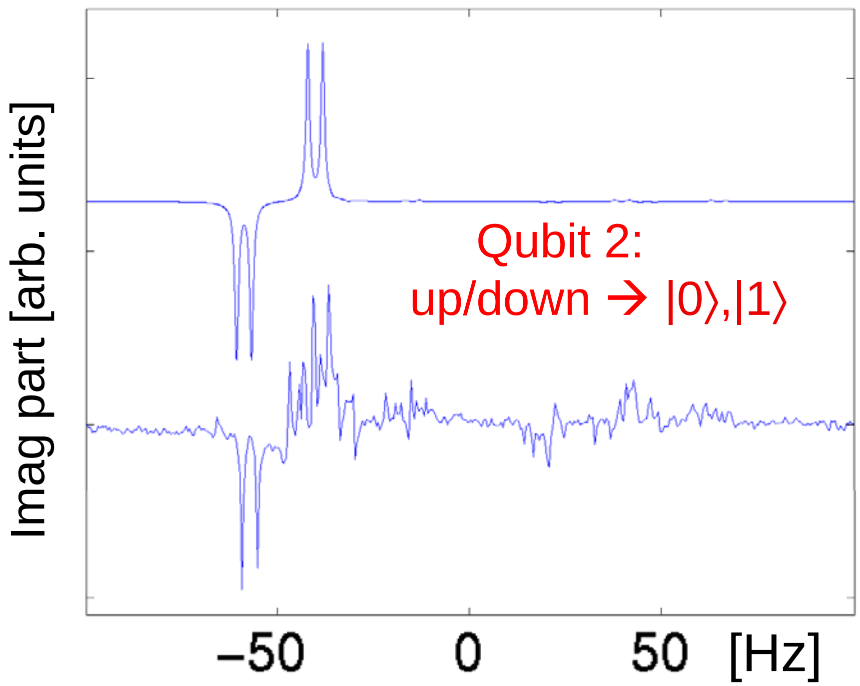
|000⟩ **0**
|010⟩ **2**
|100⟩ **4**
|110⟩ **6**

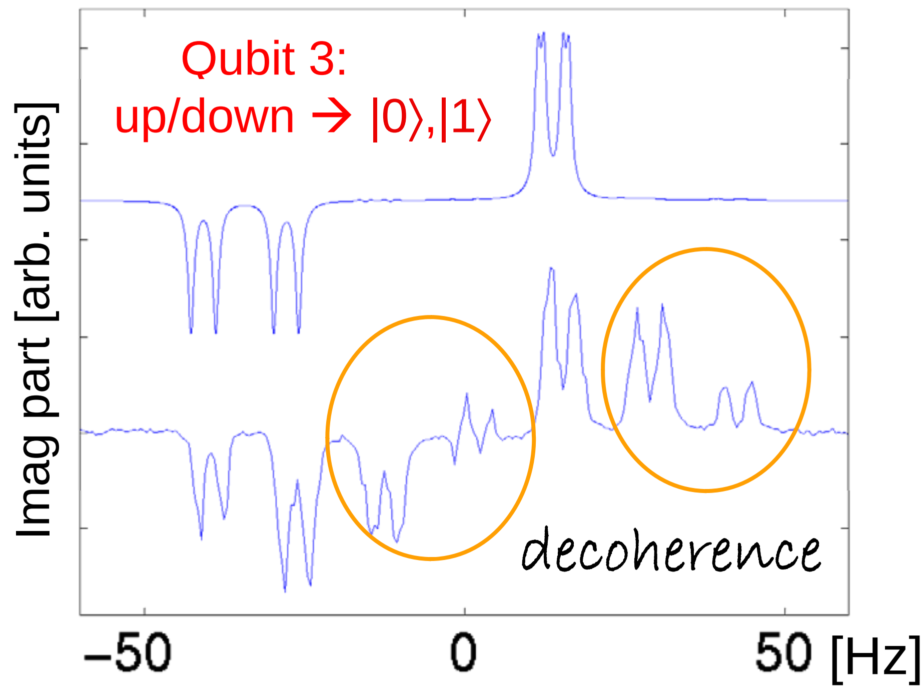
➡ $8 / r = 2$
$r = 4$ period

gcd($7^{4/2}$ - 1, 15) = 3
gcd($7^{4/2}$ + 1, 15) = 5

15 ≅ 3 x 5







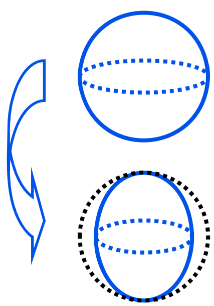
Model quantum noise (decoherence)

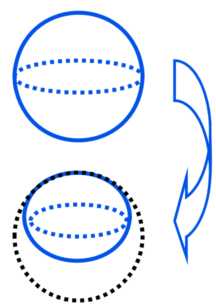
Spins interact with the environment

Decoherence

The decoherence model for 1 nuclear spin is well-described.

phase
randomization





energy
exchange

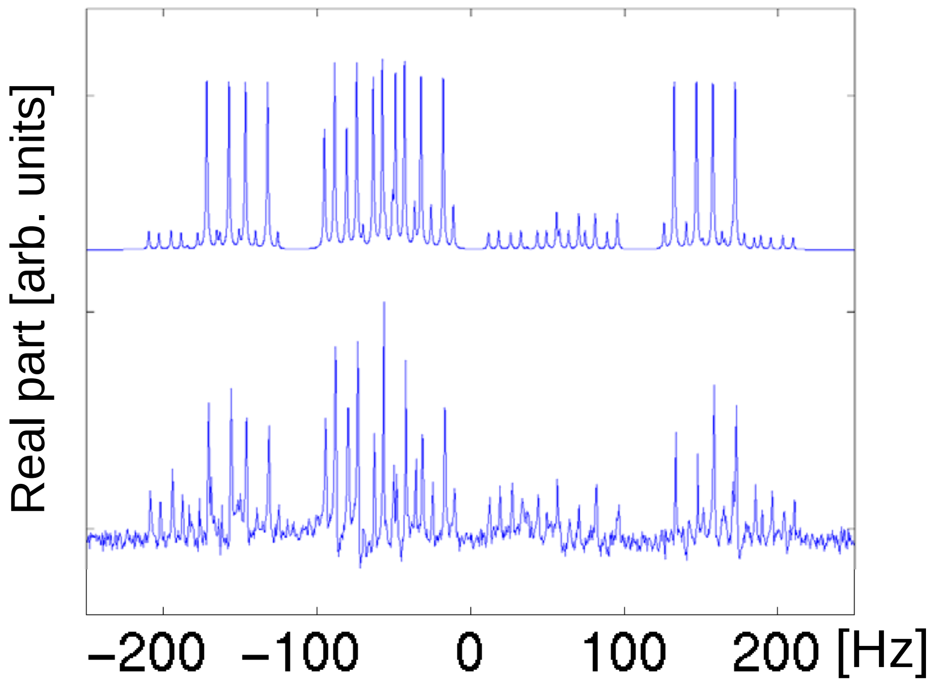
We created a workable decoherence model for 7 coupled spins.
The model is parameter free.

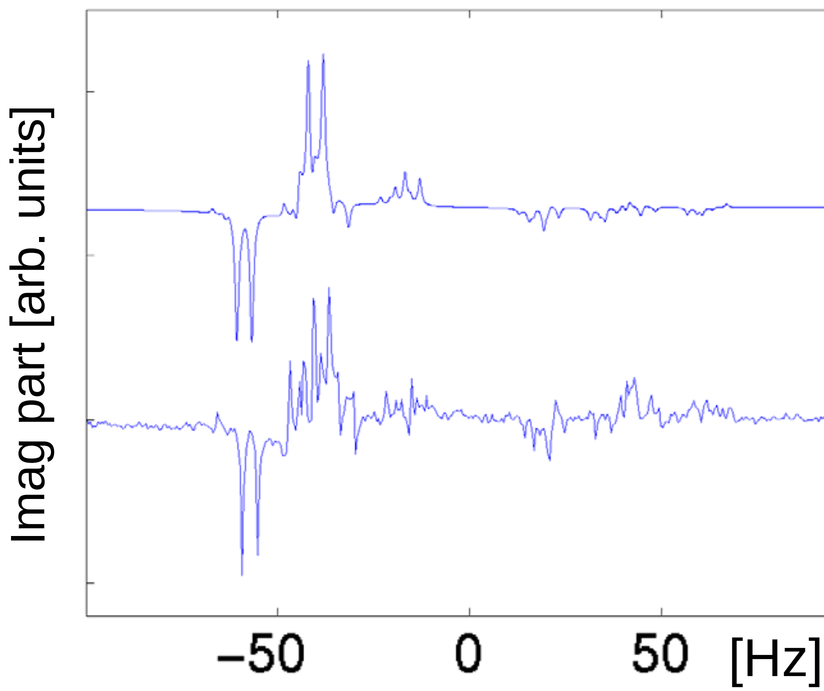
Simulation of decoherence (1)

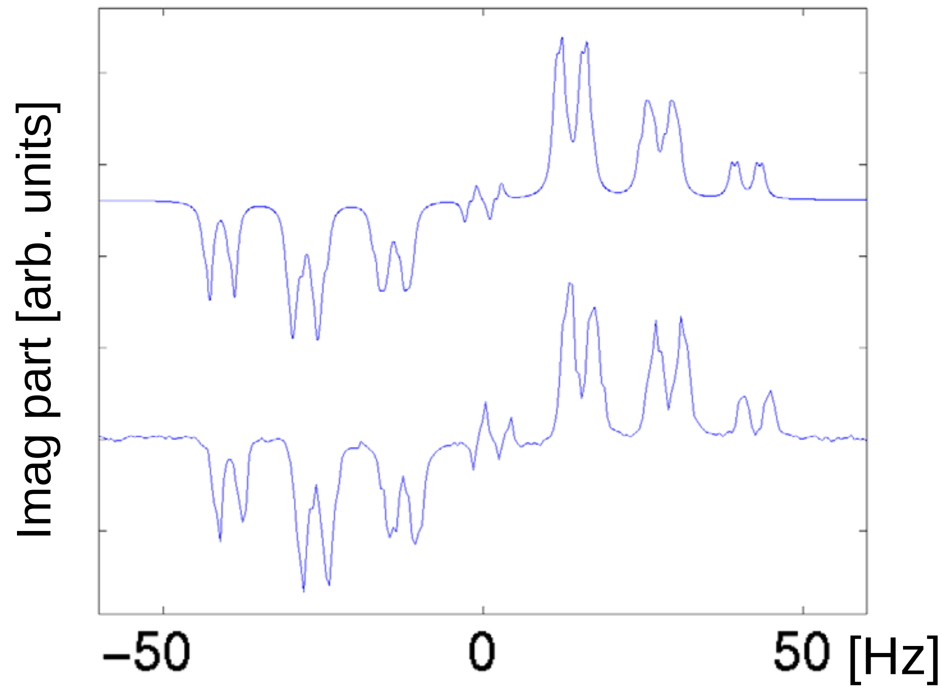
fundamental limit

hard case

decoherence can be understood and modeled







Simulation of decoherence (2)

fundamental limit

easy case

decoherence can be understood and modeled