

NMR Quantum Computing

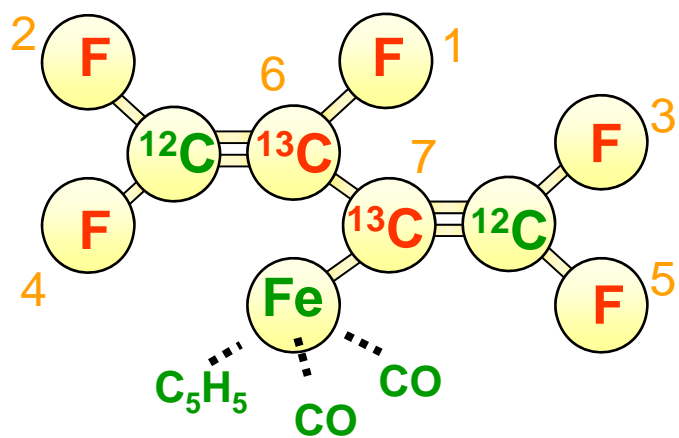


Slides courtesy of **Lieven Vandersypen**
Then: IBM Almaden, Stanford University
Now: Kavli Institute of NanoScience, TU Delft

with some annotations by Andreas Wallraff.

How to factor 15 with NMR?

perfluorobutadienyl
iron complex



red nuclei are
qubits: F, ¹³C

Goals of this lecture

Survey of NMR quantum computing

Principles of NMR QC

Techniques for qubit control

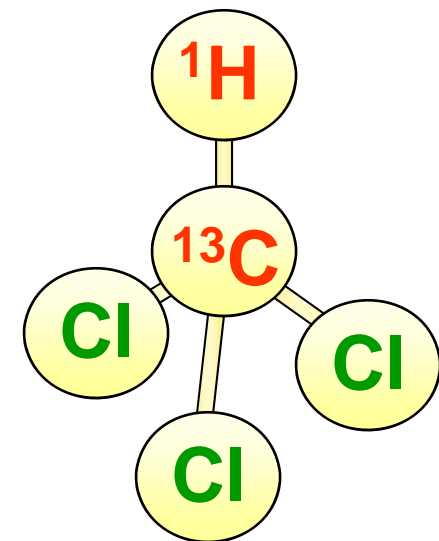
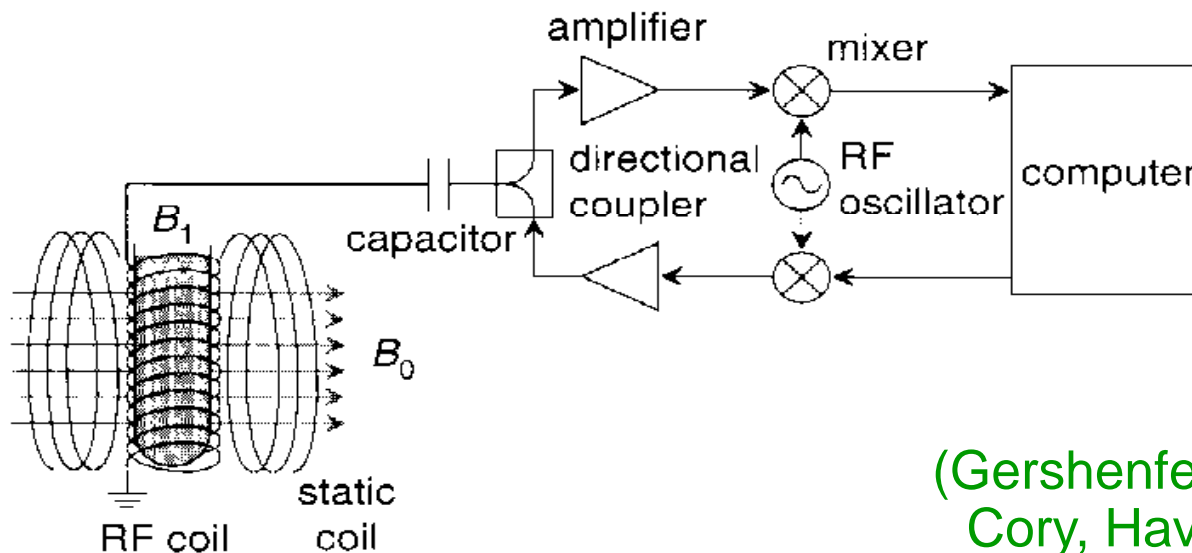
State of the art

Future of spins for QIPC

Example: factoring 15

NMR largely satisfies the DiVincenzo criteria

- ✓ Qubits: nuclear spins $\frac{1}{2}$ in B_0 field (\uparrow and \downarrow 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

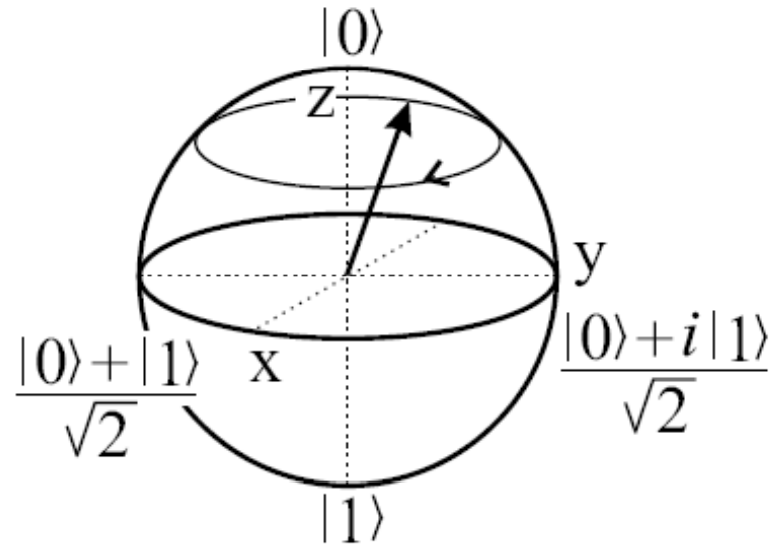
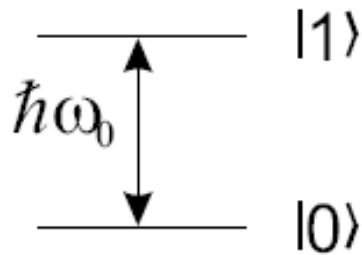


(Gershenfeld & Chuang 1997,
Cory, Havel & Fahmi 1997)

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: $\vec{I} = \hbar \vec{I}$

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

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

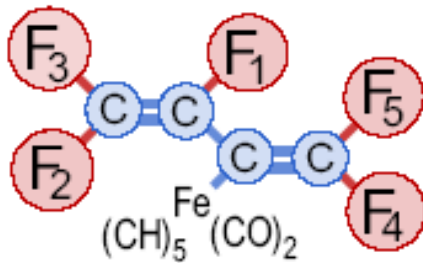
gyromagnetic (g-)factor: γ

Nuclear spin Hamiltonian

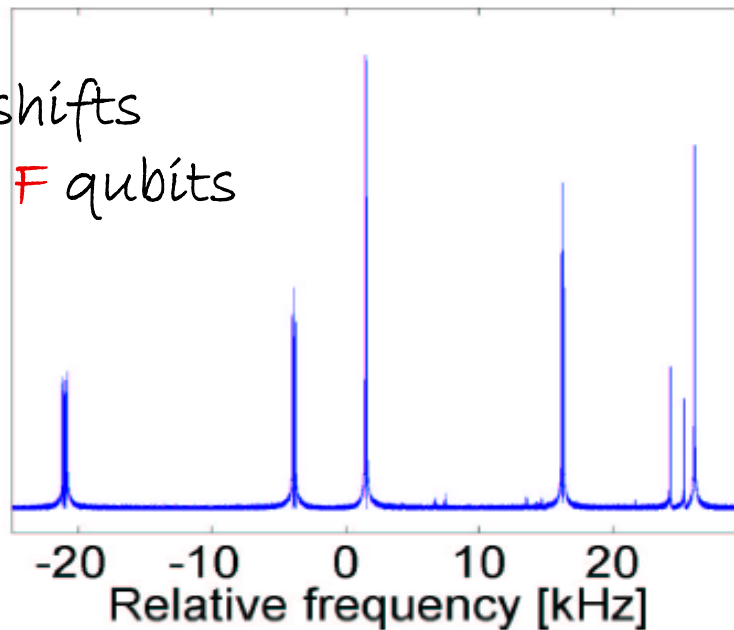
Multiple spins

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

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

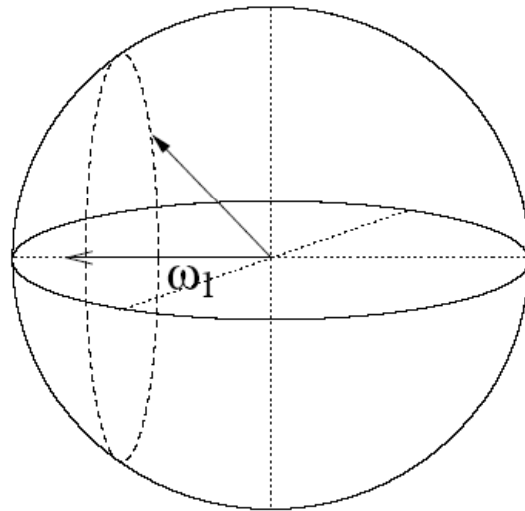


$$|\psi\rangle^{rot} = \exp(-i\omega_{rf}t I_z) |\psi\rangle$$

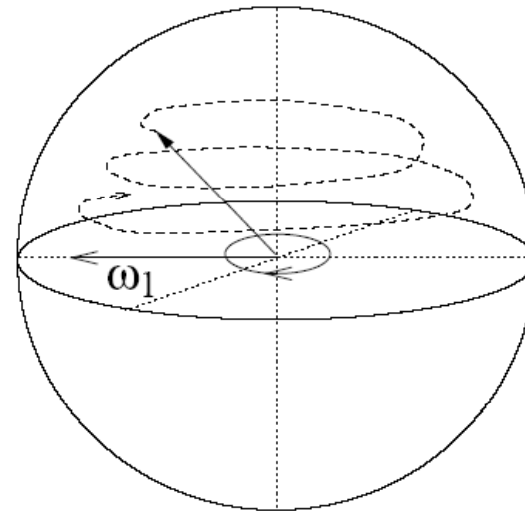
$$\mathcal{H}^{rot} = -\hbar(\omega_0 - \omega_{rf}) I_z - \hbar\omega_1 \left[\cos \phi I_x + \sin \phi I_y \right]$$

rotating wave approximation

typical strength I_x, I_y : up to 100 kHz



Rotating frame



Lab frame

Nuclear spin Hamiltonian

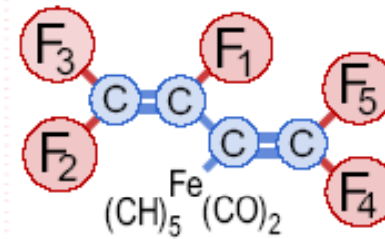
Coupled spins $J > 0$: antiferro mag.

$J < 0$: ferro-mag.

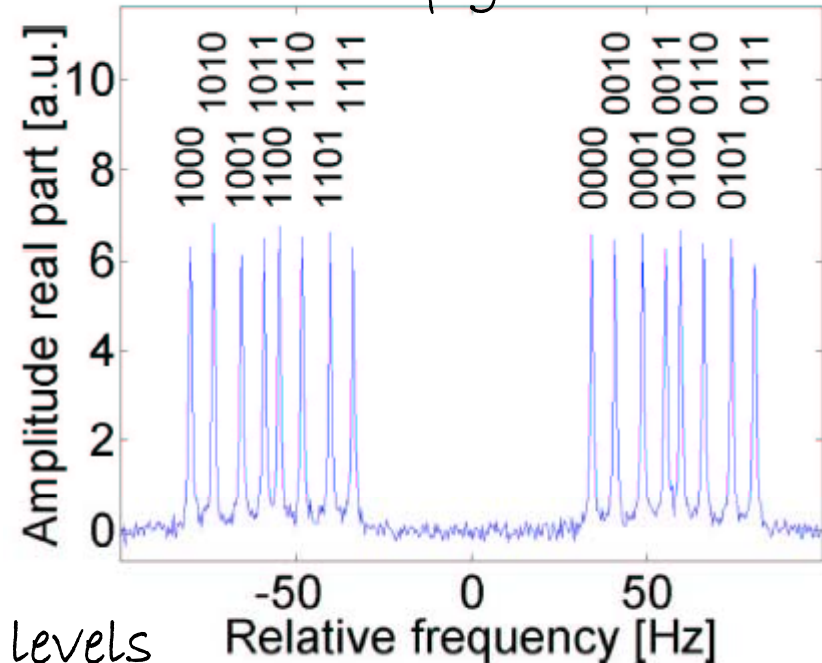
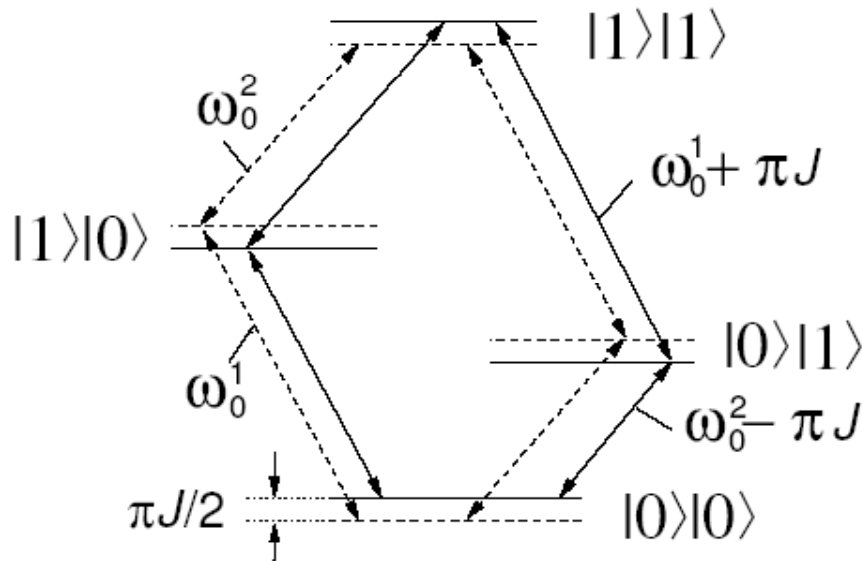
$$\mathcal{H}_J = \hbar \sum_{i < j}^n 2\pi J_{ij} I_z^i I_z^j$$

coupling term

Typical values: J up to few 100 Hz



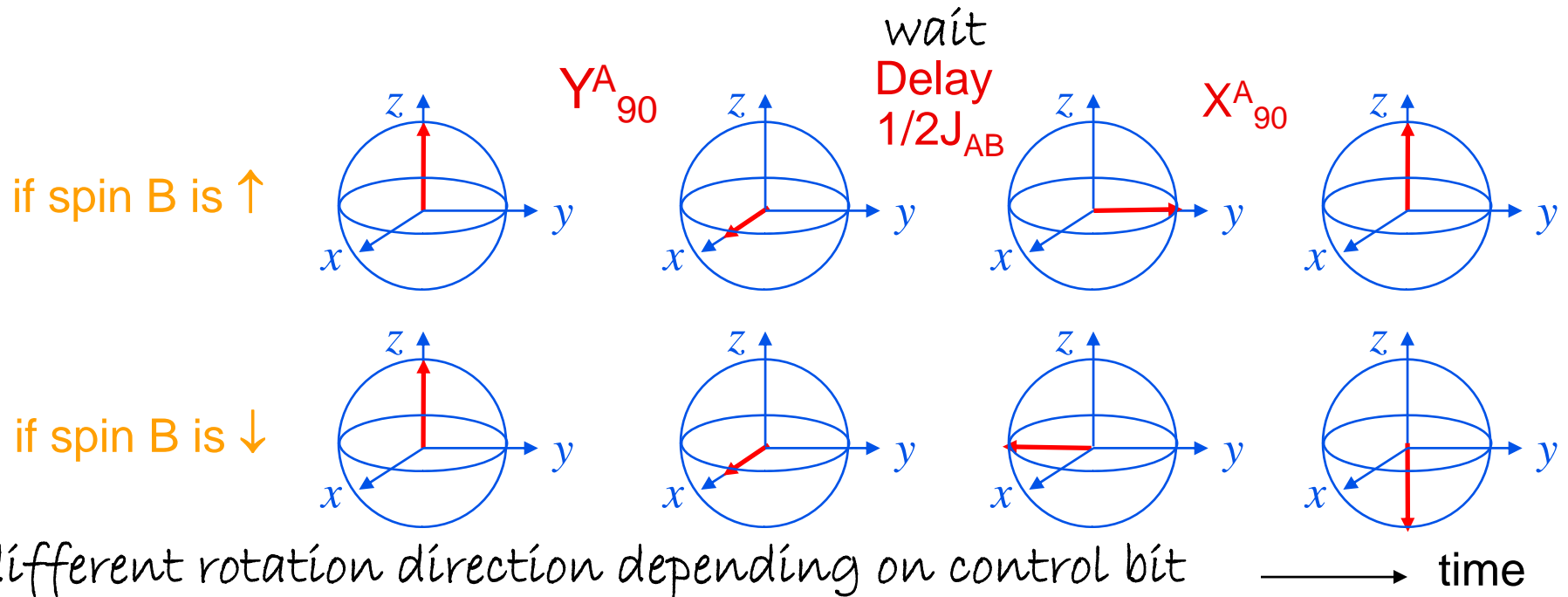
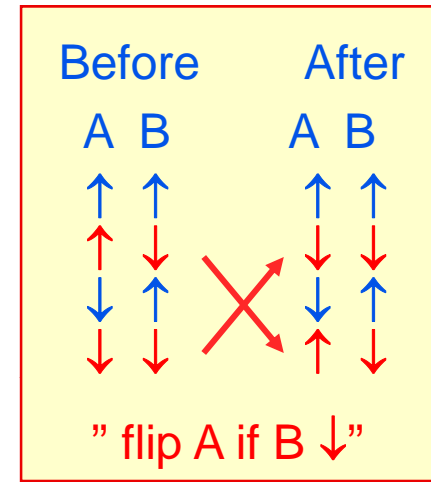
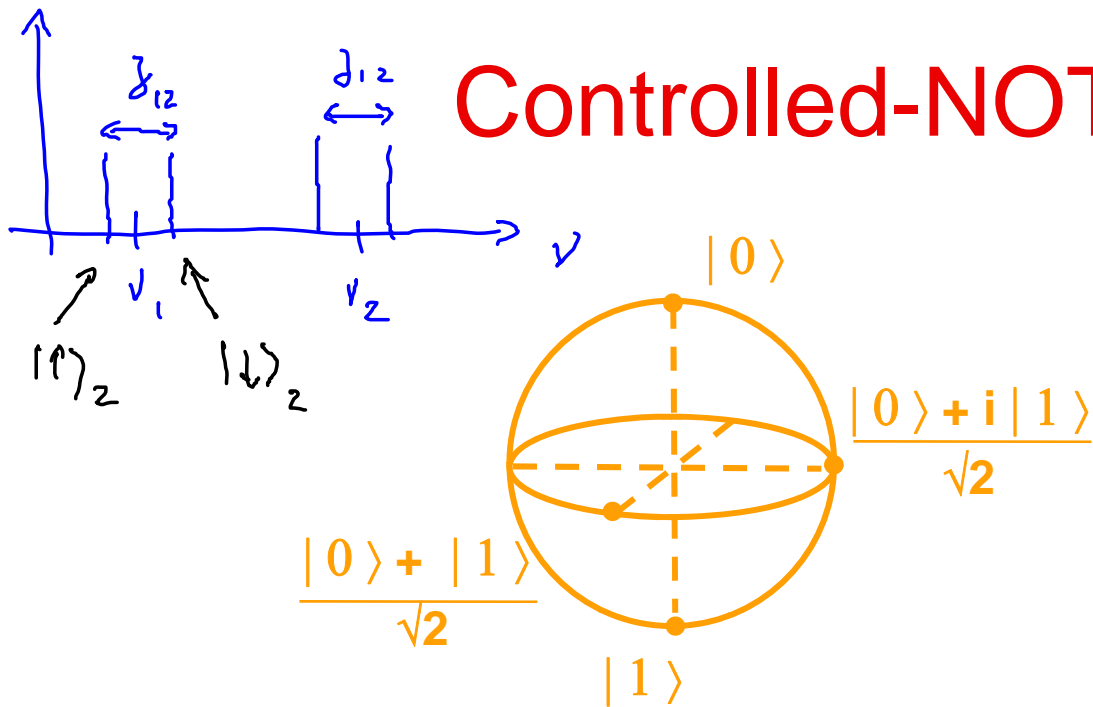
16 configurations



solid (dashed) lines are (un)coupled levels

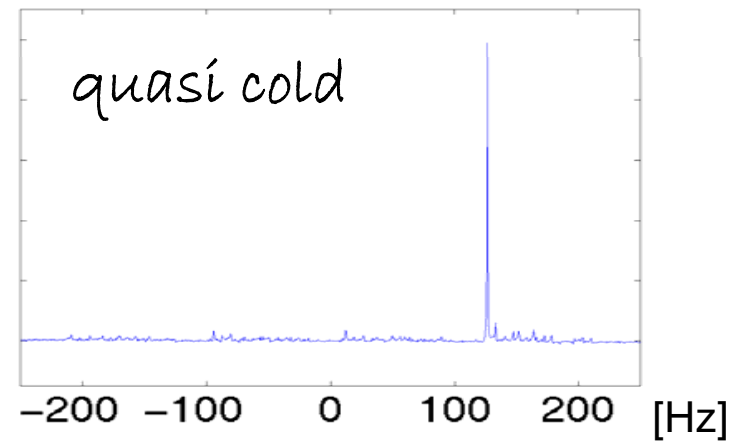
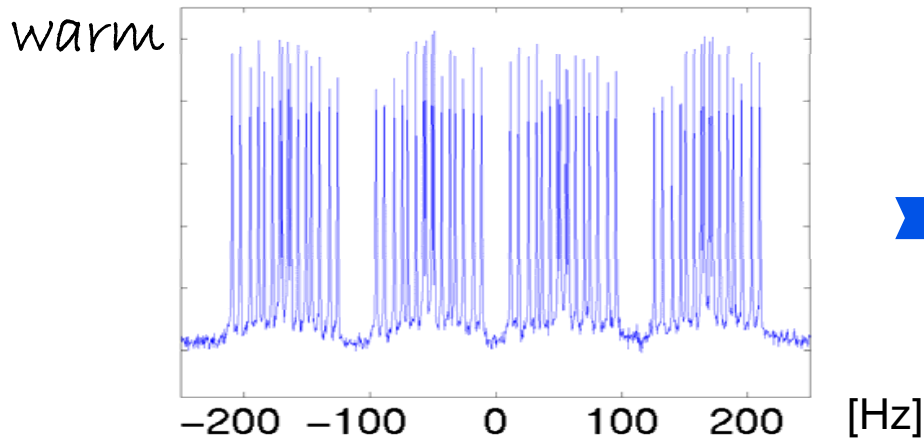
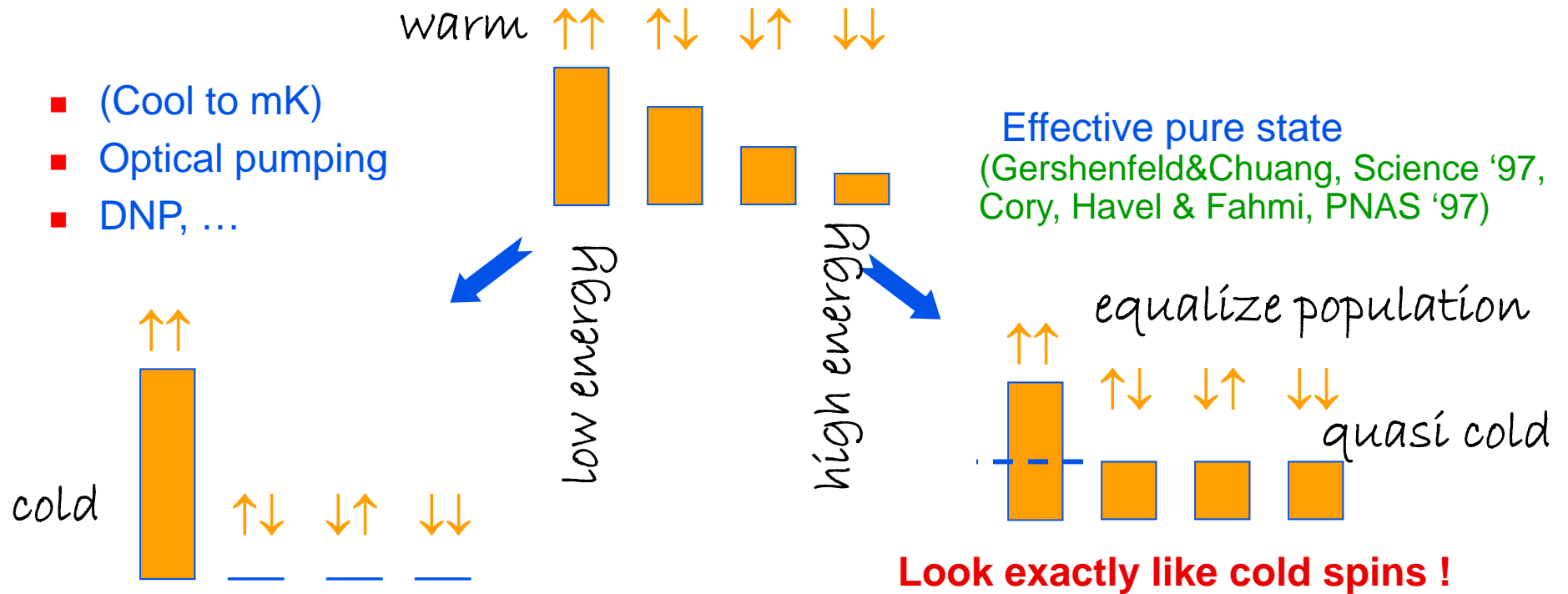
Controlled-NOT in NMR

A target bit
B control bit



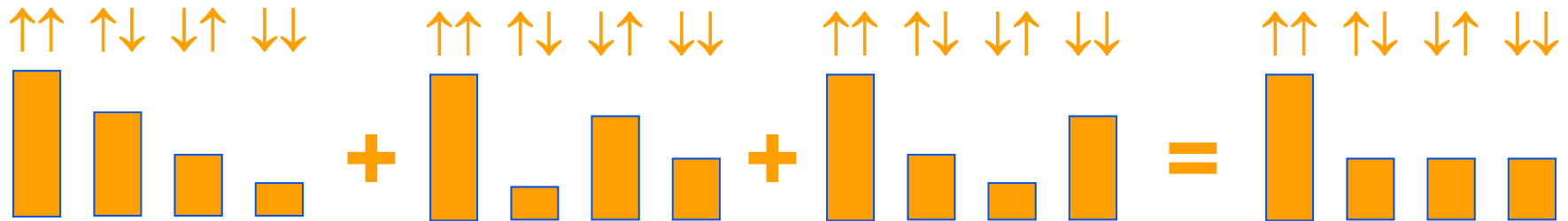
Making room temperature spins look cold

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



Effective pure state preparation

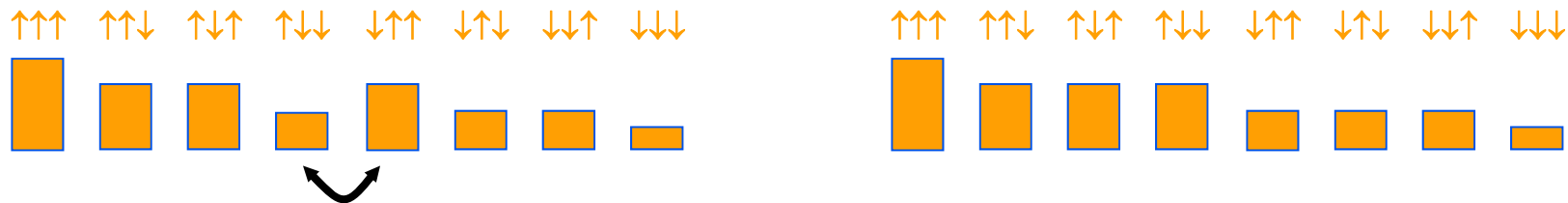
(1) Add up $2^N - 1$ experiments (Knill, Chuang, Laflamme, PRA 1998)



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

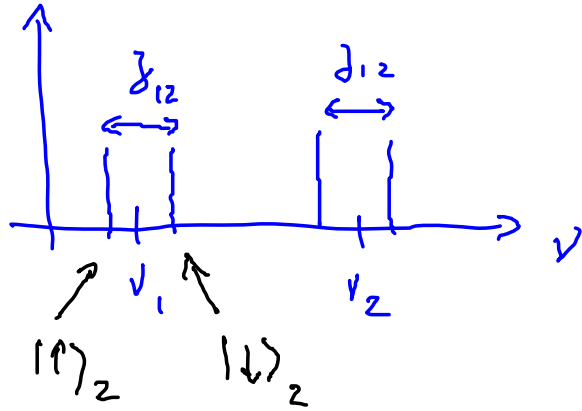
prepare equal population (on average) and look at deviations from equilibrium.

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

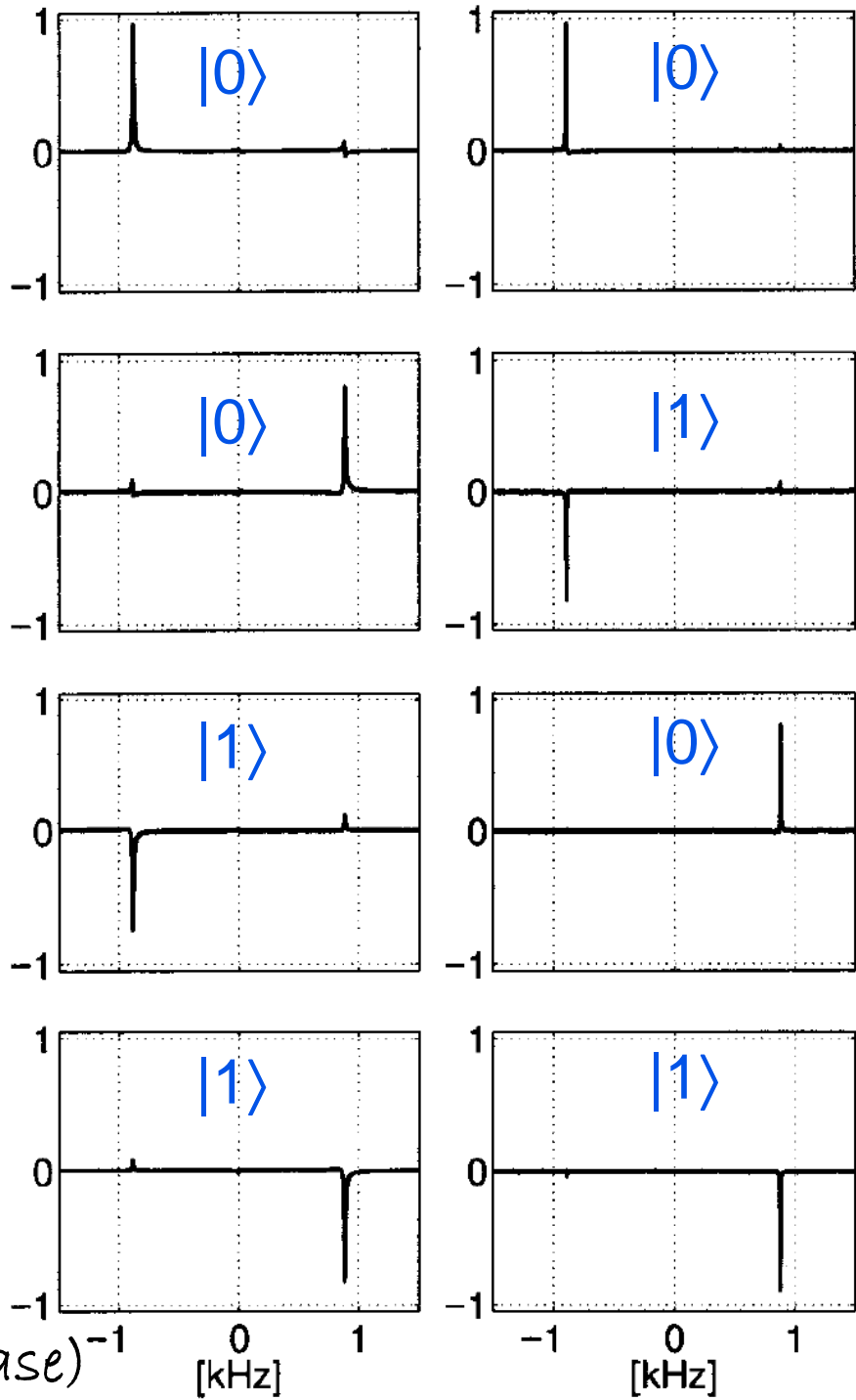
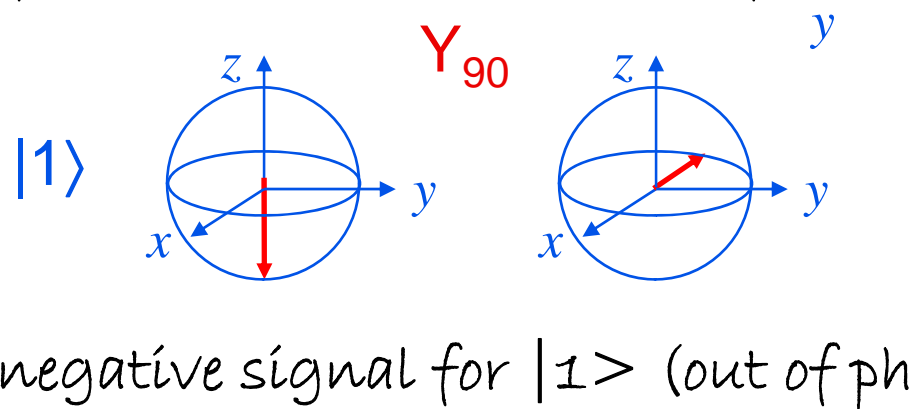
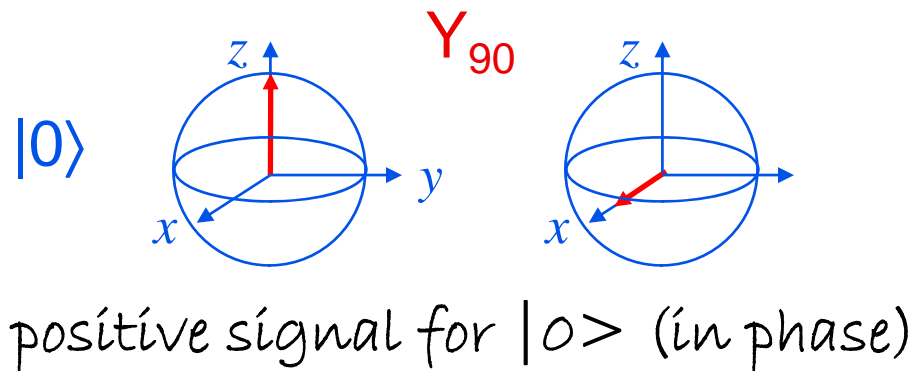


compute with qubit states that have the same energy and thus the same population.

Read-out in NMR



Phase sensitive detection



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$	

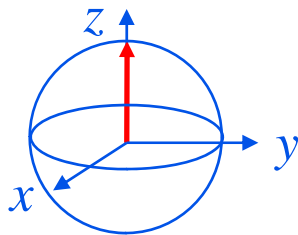
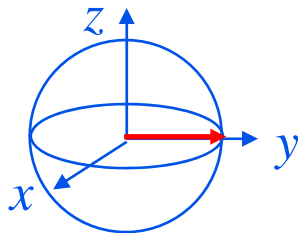
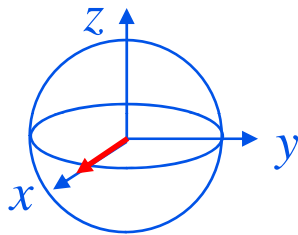


adapt algorithms if use ensemble

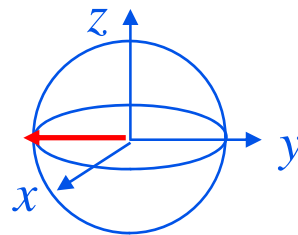
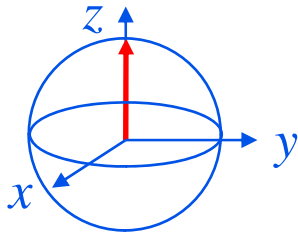
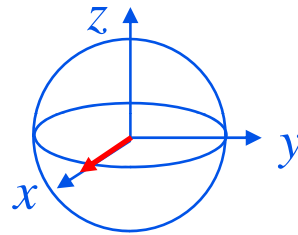
Quantum state tomography

Look at qubits from different angles

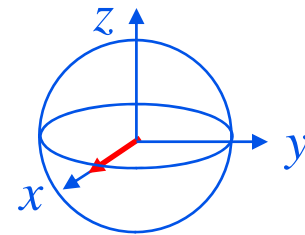
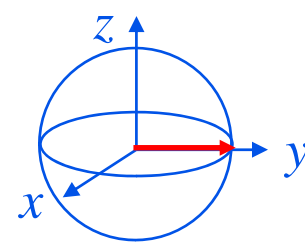
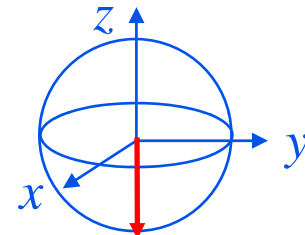
no pulse



after X_{90}



after Y_{90}



Outline

Survey of NMR quantum computing

Principles of NMR QC

➔ Techniques for qubit control

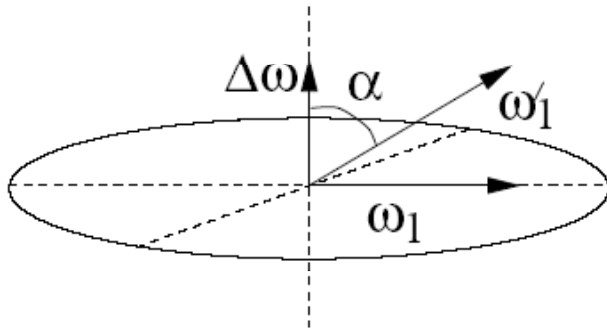
Example: factoring 15

State of the art

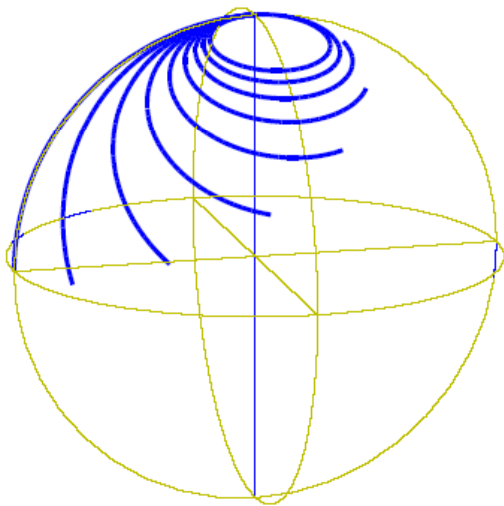
Outlook

Off-resonance pulses and spin-selectivity

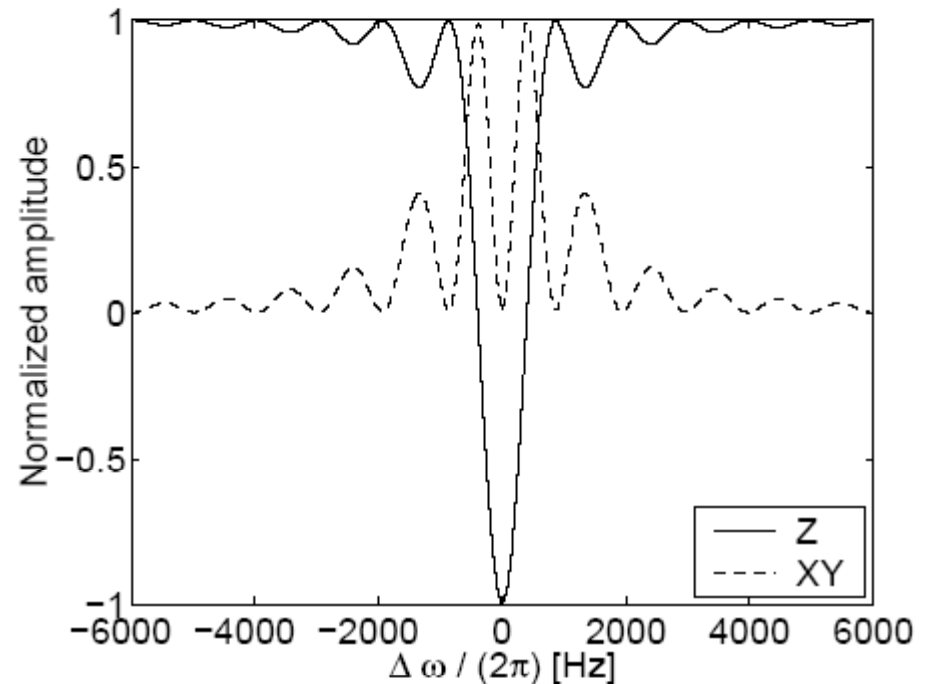
$$\mathcal{H}^{rot} = -\hbar (\omega_0 - \omega_{rf}) I_z - \hbar \omega_1 \left[\cos \phi I_x + \sin \phi I_y \right]$$



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

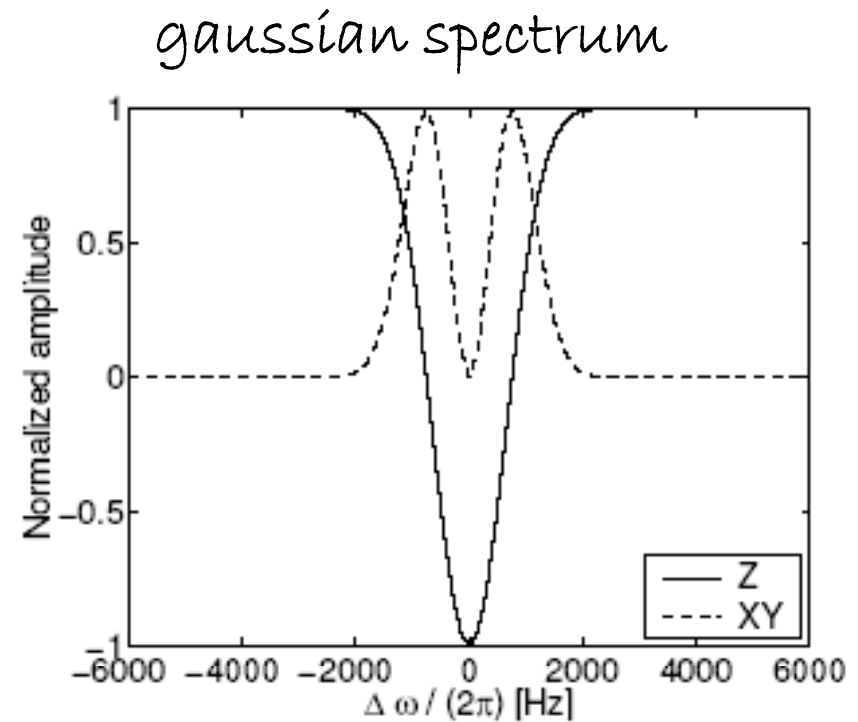
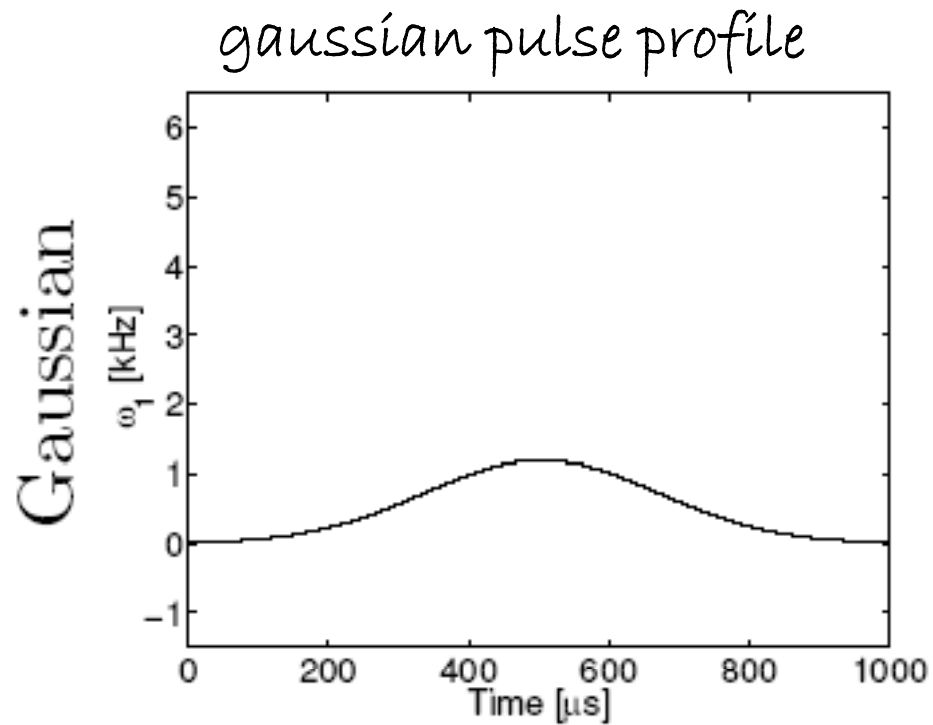


spectral content of a square pulse



may induce transitions in other qubits

Pulse shaping for improved spin-selectivity



less cross-talk

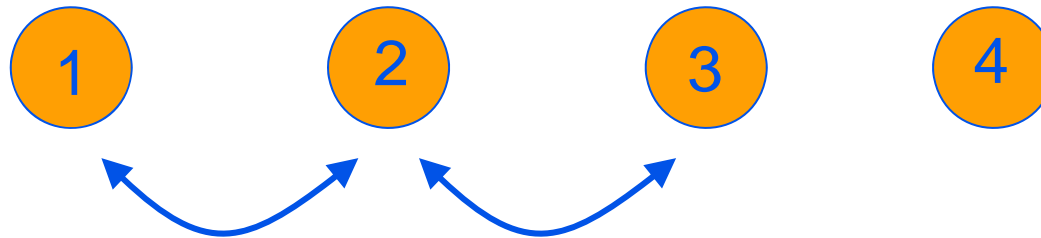
Missing coupling terms: Swap

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

Missing couplings: swap states along qubit network

$$\text{SWAP}_{12} = \text{CNOT}_{12} \text{CNOT}_{21} \text{CNOT}_{12}$$

*as discussed
in exercise class*

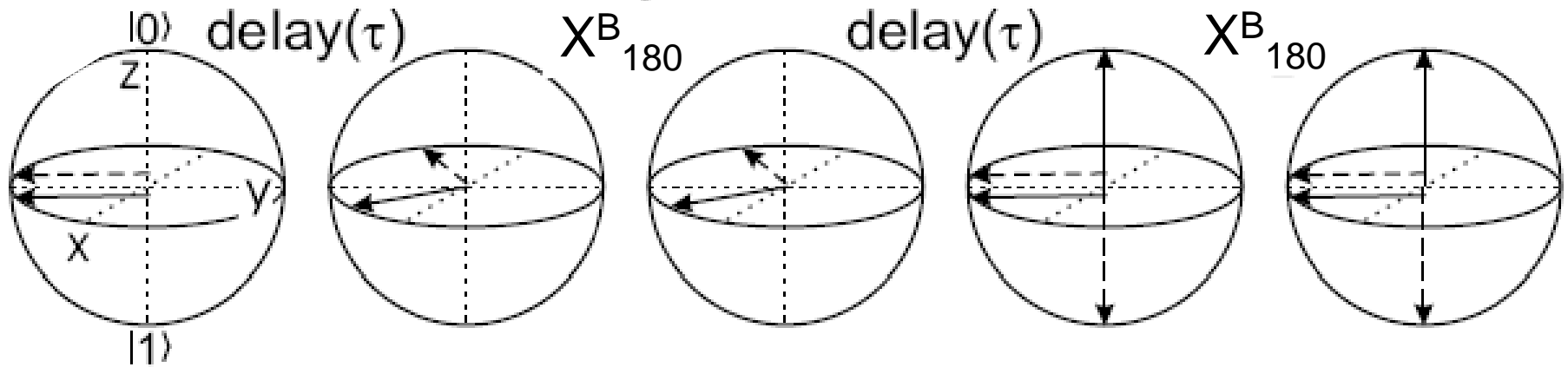


“only” a linear overhead ...

Undesired couplings: refocus

remove effect of coupling *during delay times*

opt. 1: act on qubit B



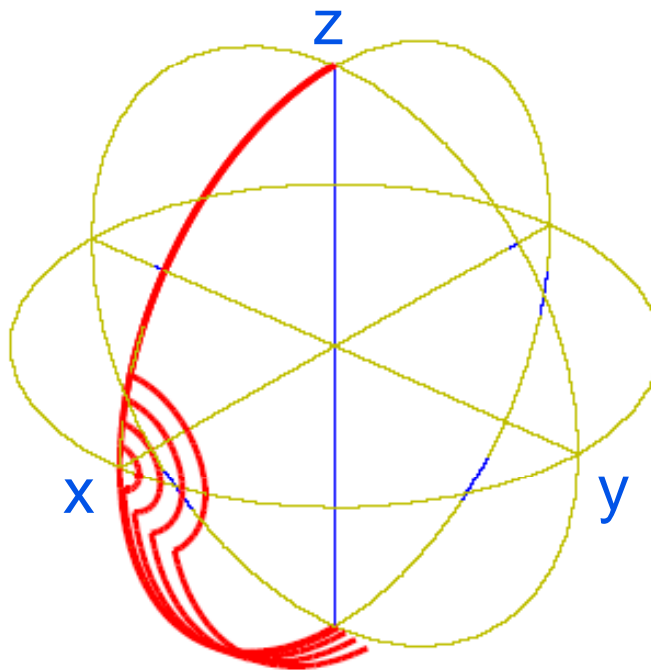
opt. 2: act on qubit A

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

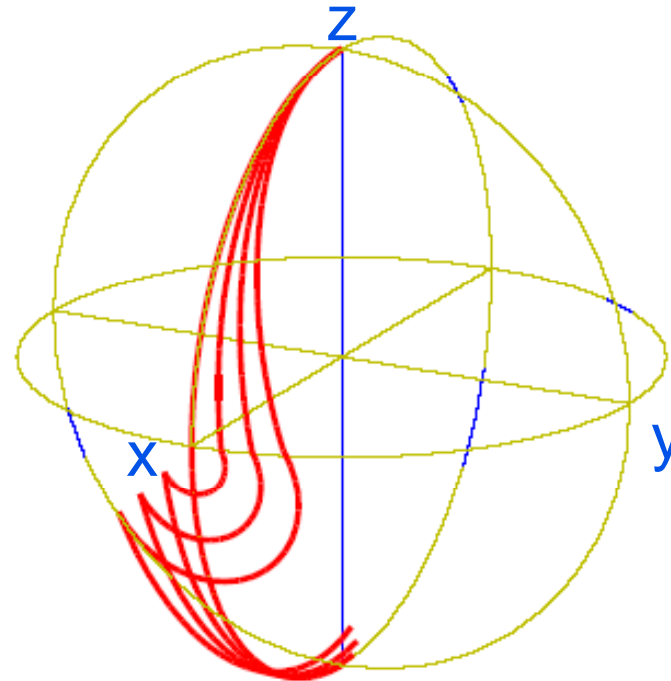
Composite pulses

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

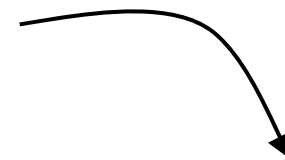
Molecule selection

A quantum computer is a *known* molecule.

Its desired properties are:

- spins 1/2 (^1H , ^{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, ...

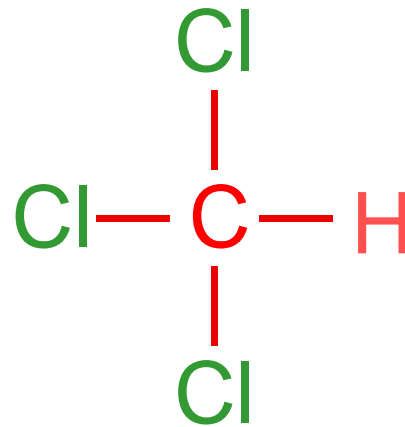


required to make
spins of same
type addressable

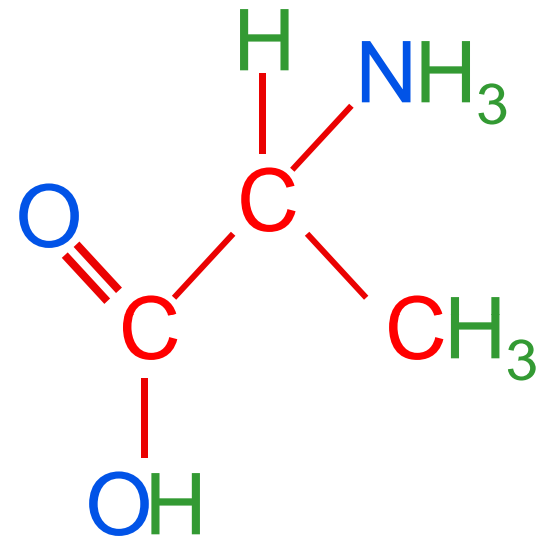
Quantum computer molecules (1)

red nuclei are used
as qubits:

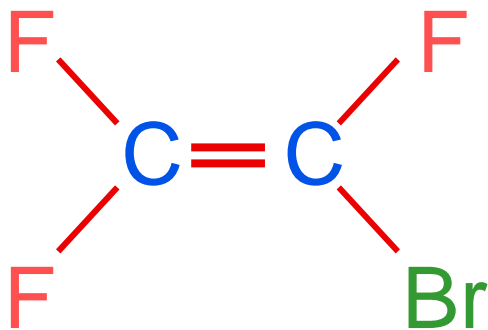
Grover / Deutsch-Jozsa



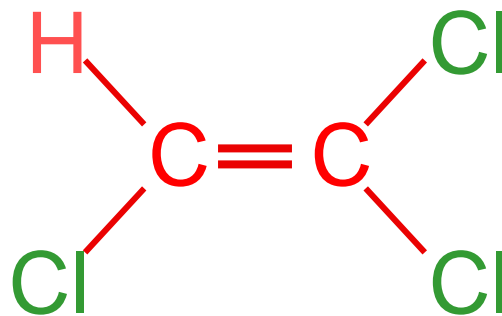
Q. Error correction



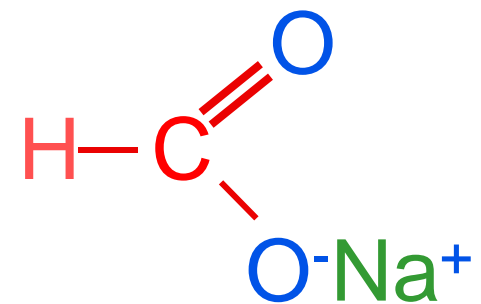
Logical labeling / Grover



Teleportation

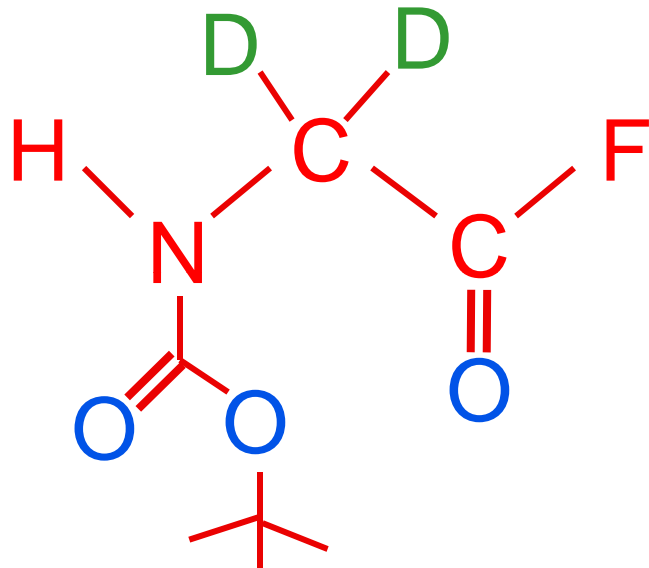


Q. Error Detection

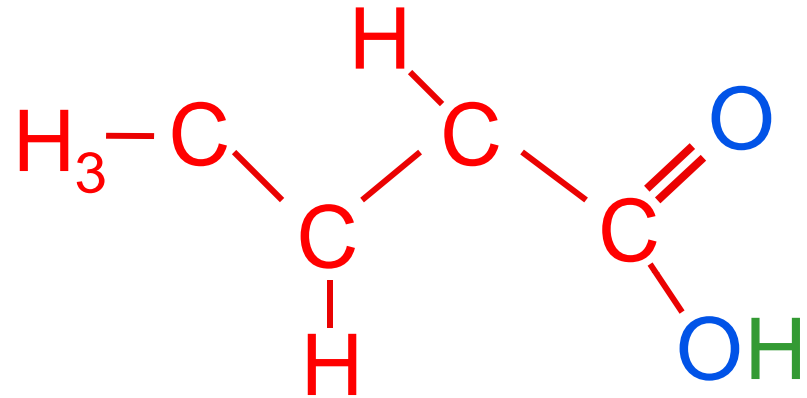


Quantum computer molecules (2)

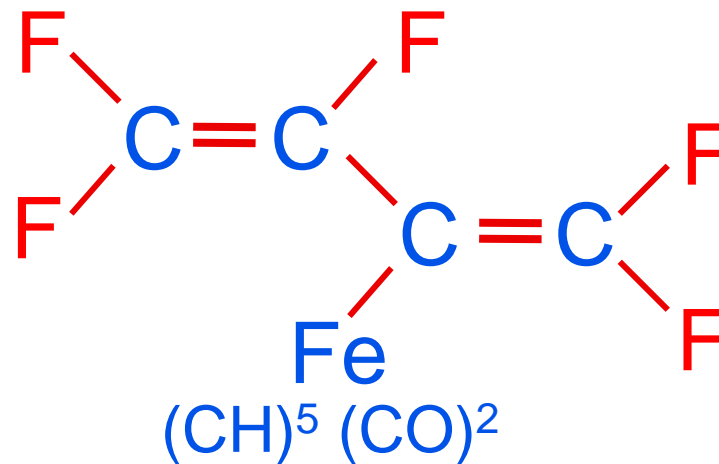
Deutsch-Jozsa



7-spin coherence



Order-finding



Outline

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Principles of NMR QC

Techniques for qubit control

Example: factoring 15

→ { State of the art
Outlook

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 $\sim 1 / 2^n$ [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 coupling during RF pulses

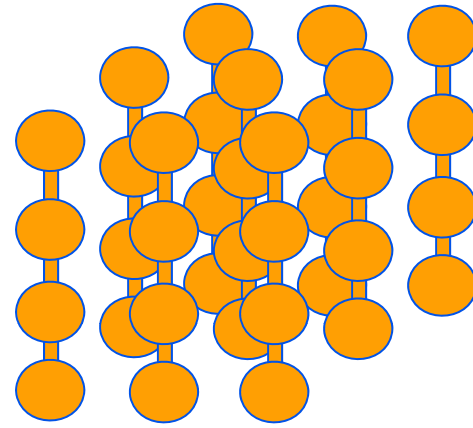
Finally

decoherence

Solid-state NMR ?

molecules in
solid matrix

Cory et al

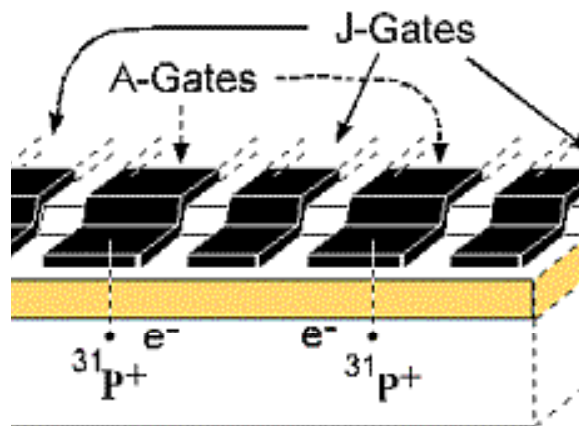


Yamaguchi & Yamamoto, 2000

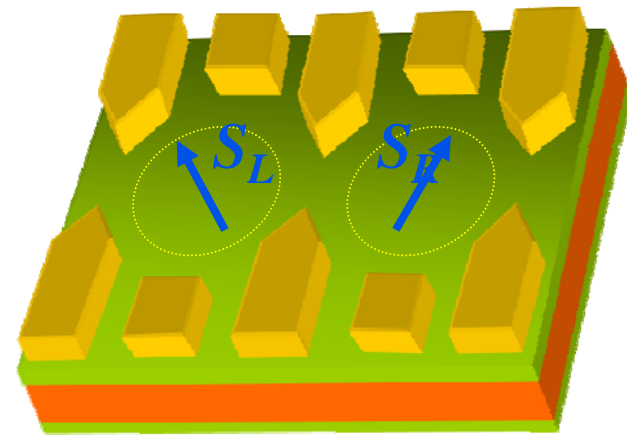
$$\mathcal{H}_J = \hbar \sum_{i < j} 2\pi J_{ij} \vec{I}^i \cdot \vec{I}^j = \hbar \sum_{i < j} 2\pi J_{ij} (I_x^i I_x^j + I_y^i I_y^j + I_z^i I_z^j)$$

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

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 .

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

↑ ↑
coprime with 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: $\sim e^{L/3}$

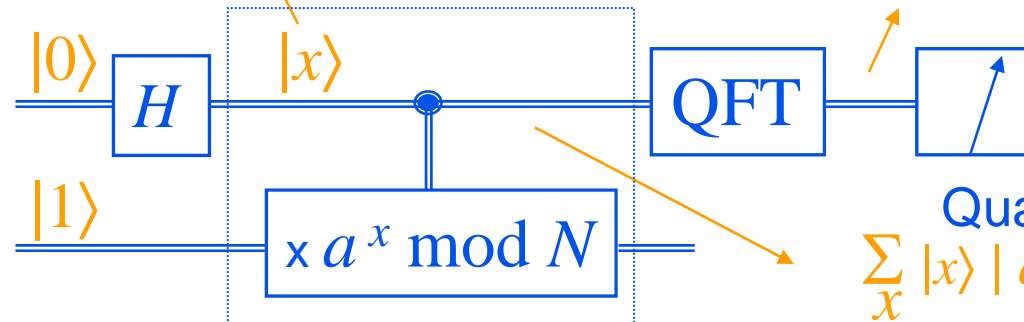
Widely used crypto systems (RSA) would become insecure.

Factoring 15 - schematic

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

$$\sum_k |k2L/r\rangle \text{ Interference}$$

2 L bits
3 qubits
 $L = \log_2(15)$
4 qubits

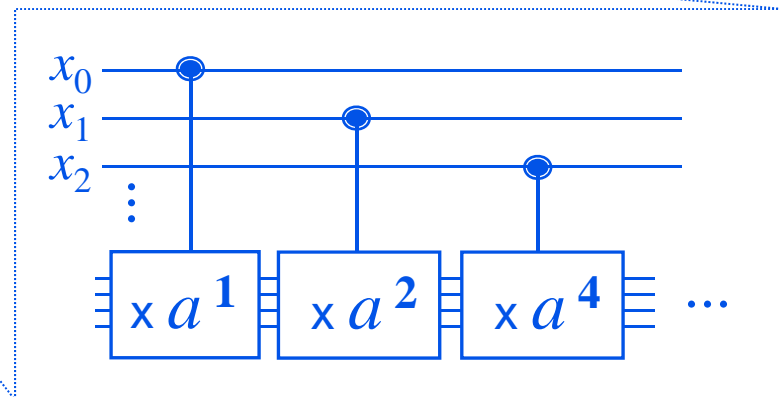


$$\sum_x |x\rangle |a^x \text{ mod } 15\rangle$$

Quantum parallelism

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

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



$a = 4, 11 \Rightarrow a^2 \text{ mod } 15 = 1 \Rightarrow$ “easy” case period 2

$a = 2, 7, 8, 13 \Rightarrow a^4 \text{ mod } 15 = 1 \Rightarrow$ “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

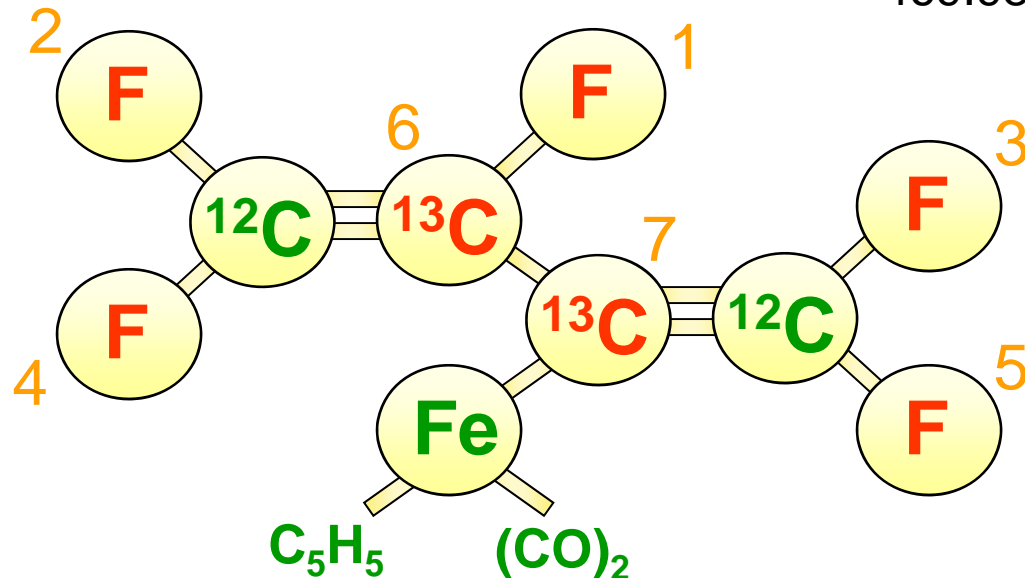
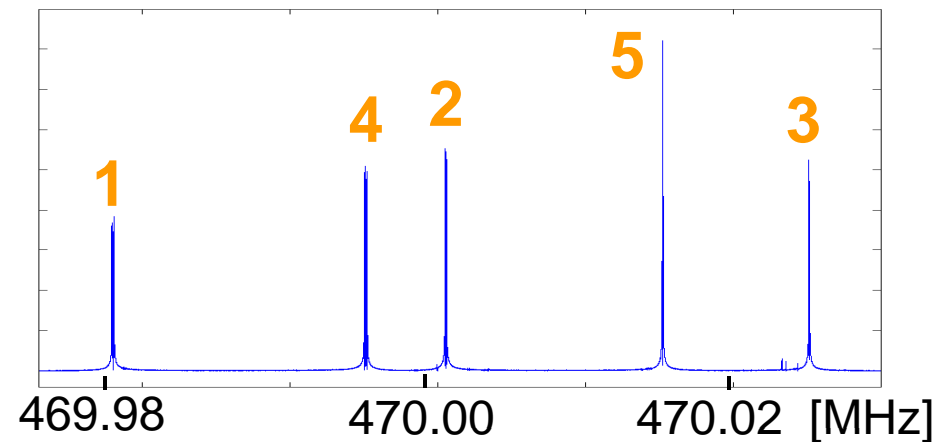
$$a = 11$$

$$\begin{aligned}
 |\psi_3\rangle &= |0\rangle |0\rangle + |1\rangle |2\rangle + |2\rangle |0\rangle + |3\rangle |2\rangle + |4\rangle |0\rangle + |5\rangle |2\rangle + |6\rangle |0\rangle + |7\rangle |2\rangle \\
 &= (|0\rangle + |2\rangle + |4\rangle + |6\rangle) |0\rangle + (|1\rangle + |3\rangle + |5\rangle + |7\rangle) |2\rangle \text{ after mod exp}
 \end{aligned}$$

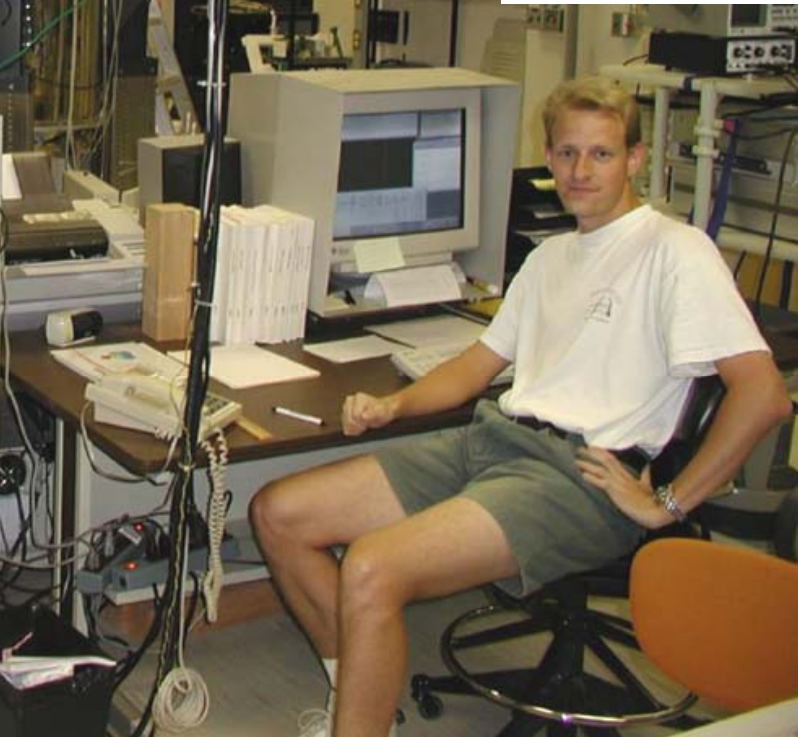
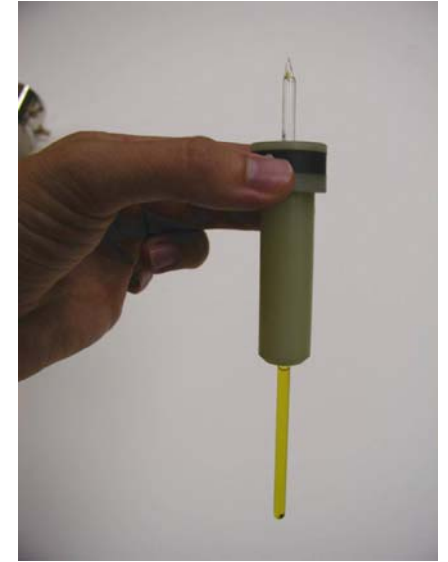
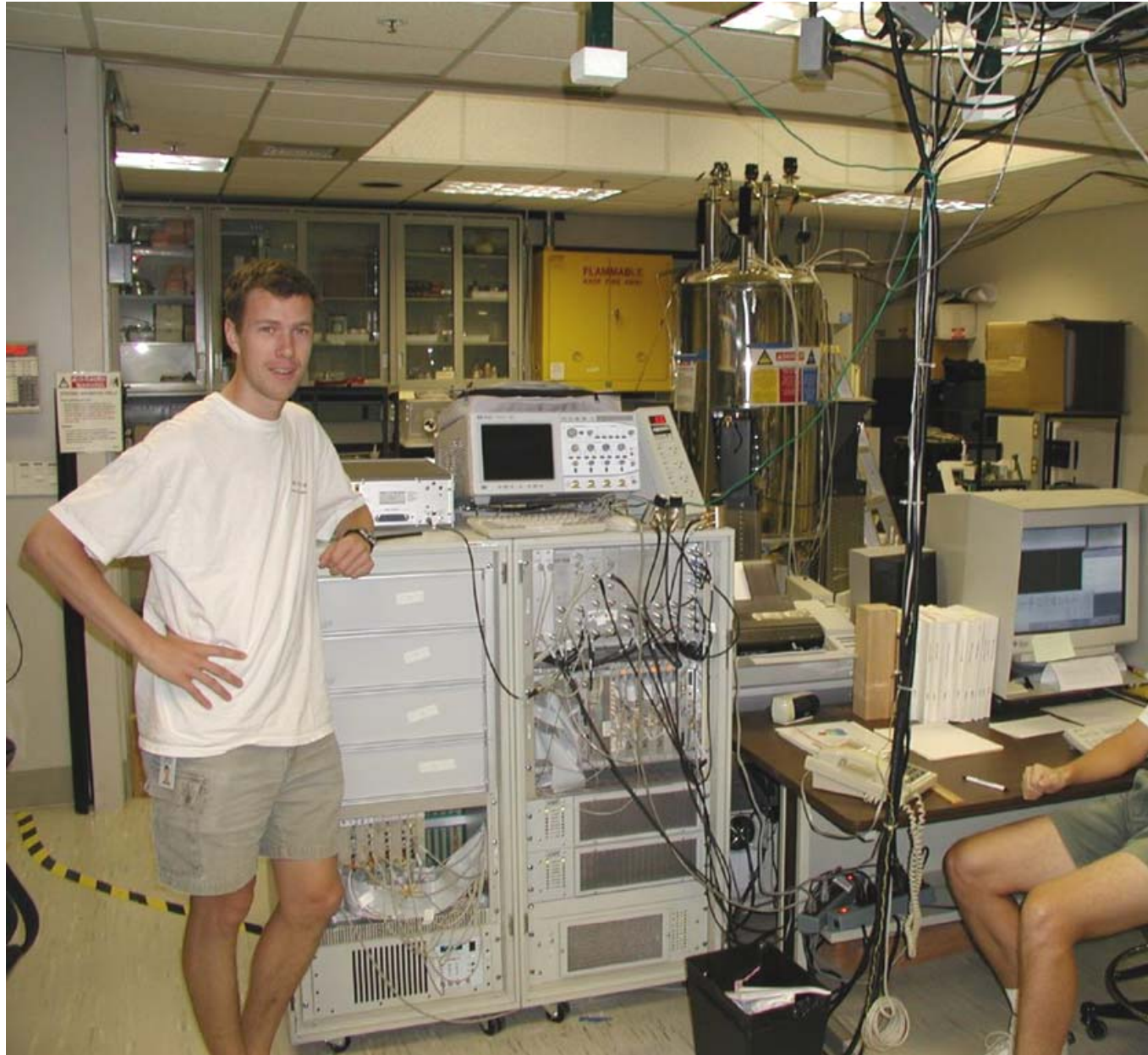
$$|\psi_4\rangle = (|0\rangle + |4\rangle) |0\rangle + (|0\rangle - |4\rangle) |2\rangle \text{ after QFT}$$

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

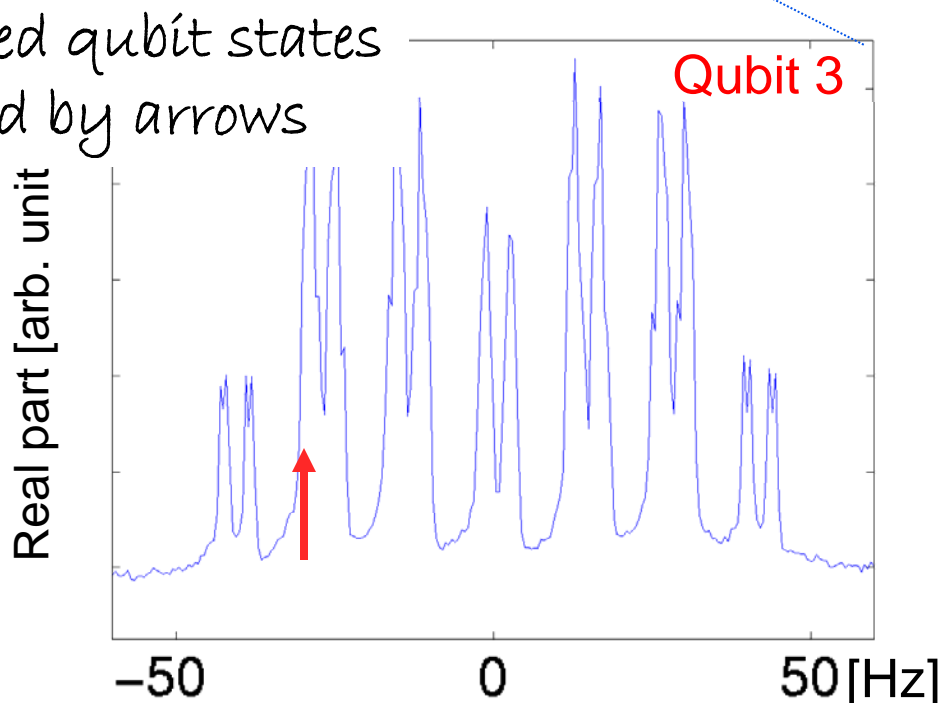
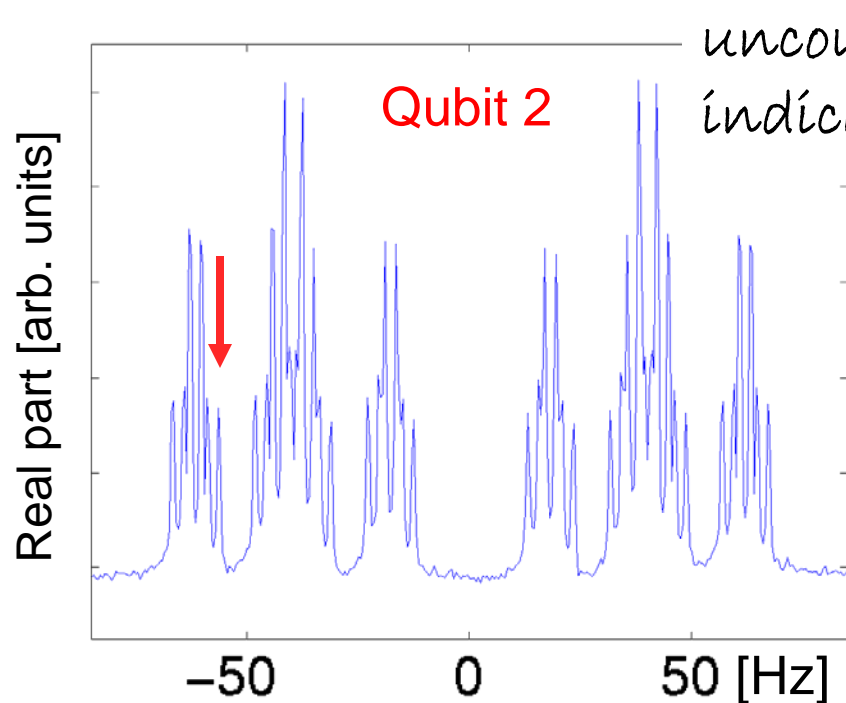
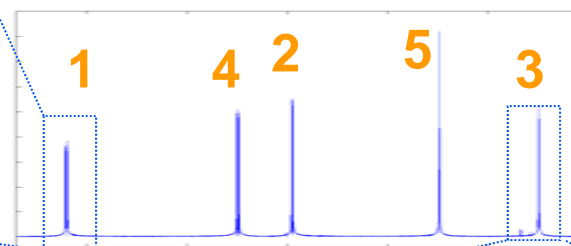
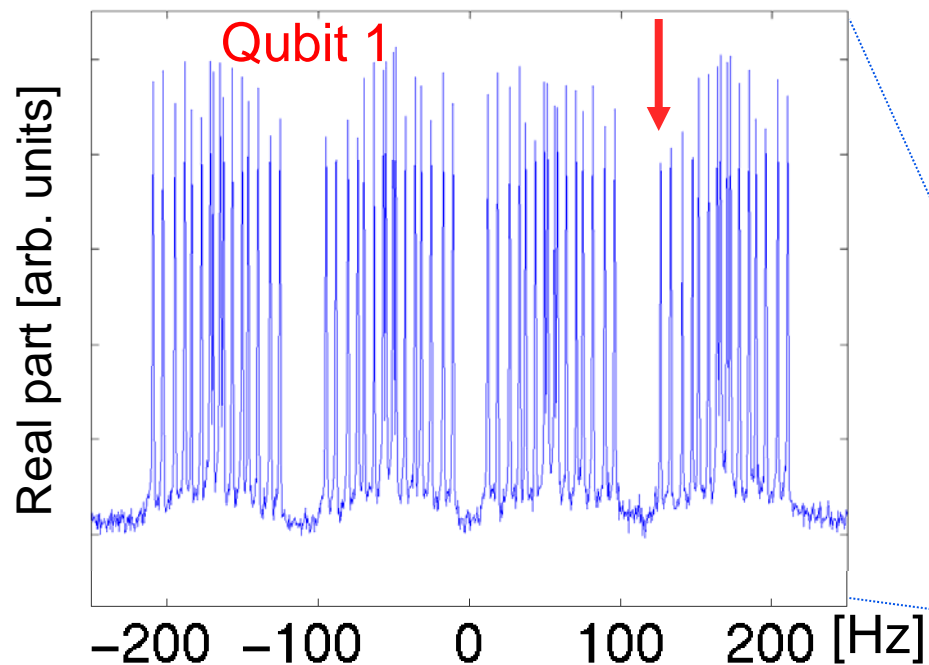


- Larmor frequencies
 - 470 MHz for ^{19}F ~ 25 mK
 - 125 MHz for ^{13}C
- J - couplings: 2 - 220 Hz
- coherence times: 1.3 - 2 s



Thermal Equilibrium Spectra

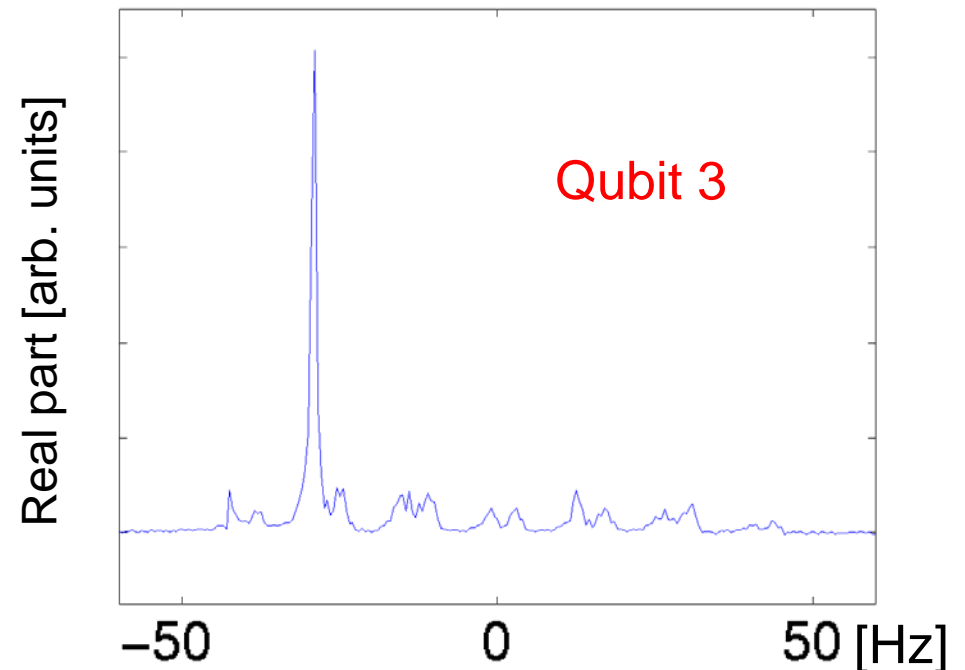
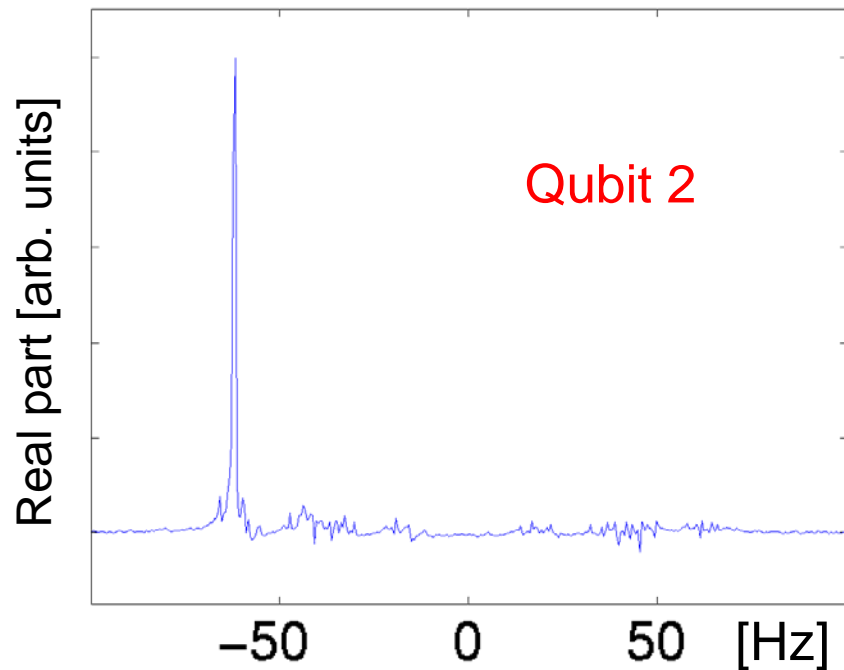
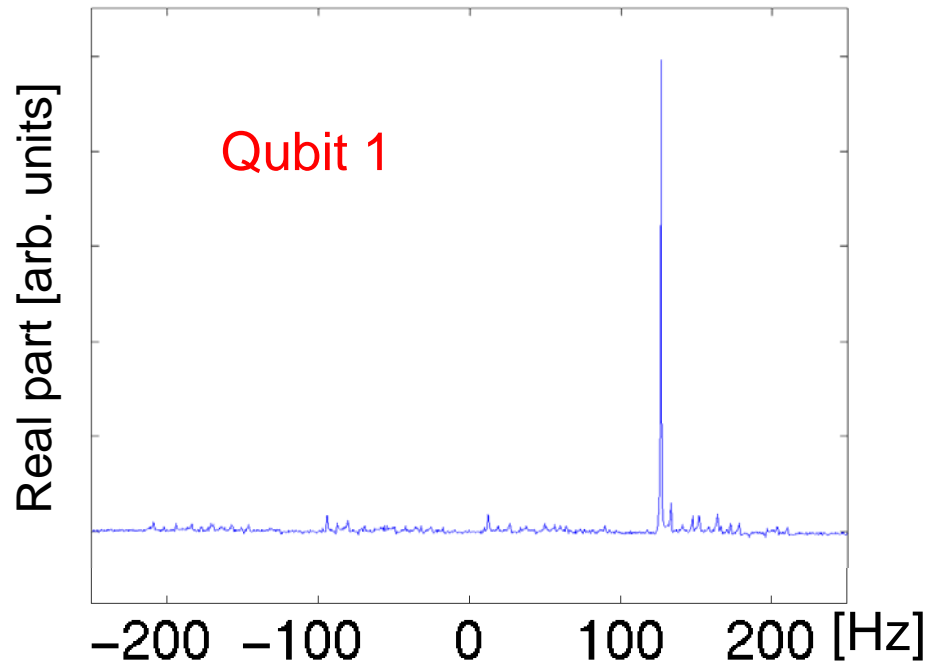
- line splitting due to J -coupling
- all lines present



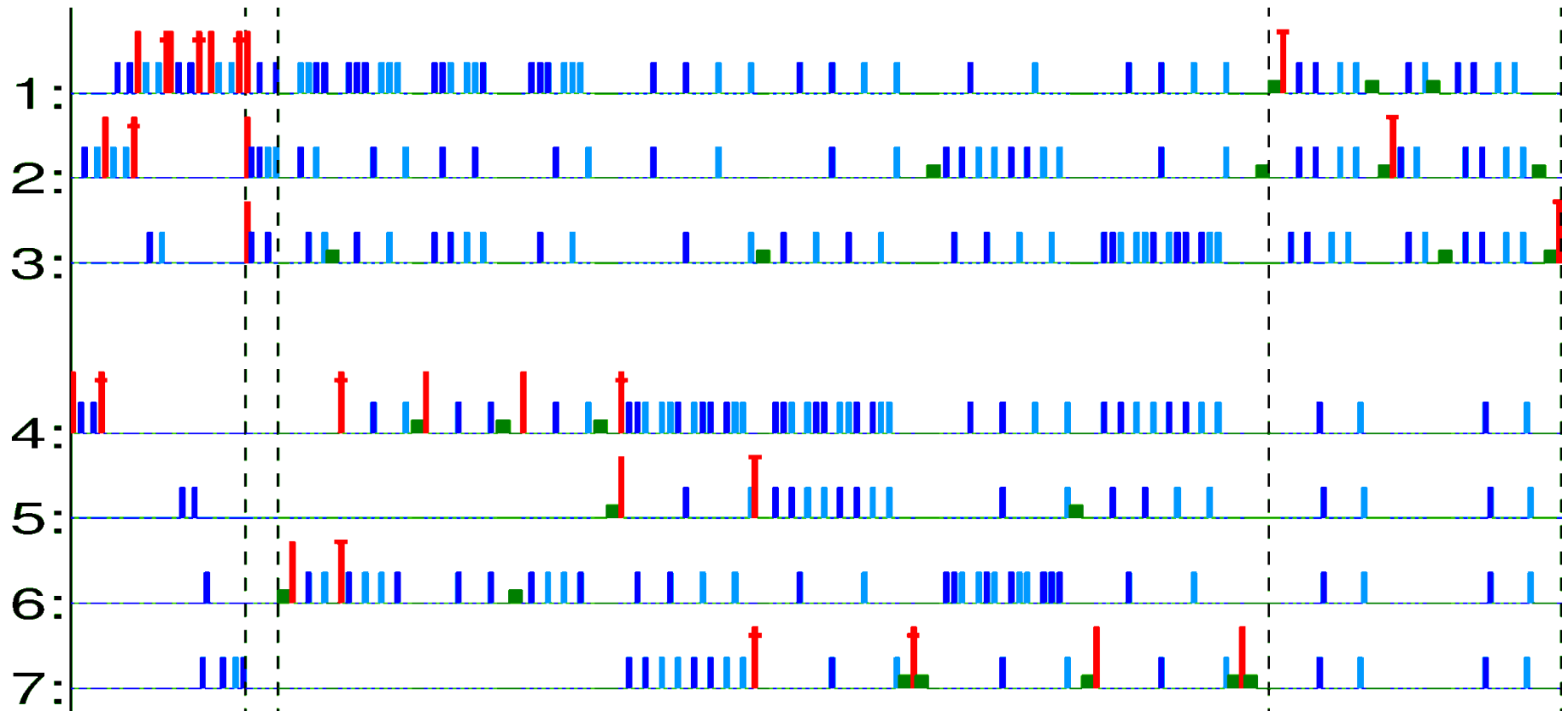
Spectra after state initialization

- only the $|00 \dots 0\rangle$ line remains
- the other lines are averaged away by adding up multiple experiments

RT spins appear cold!



Pulse sequence ($a=7$)

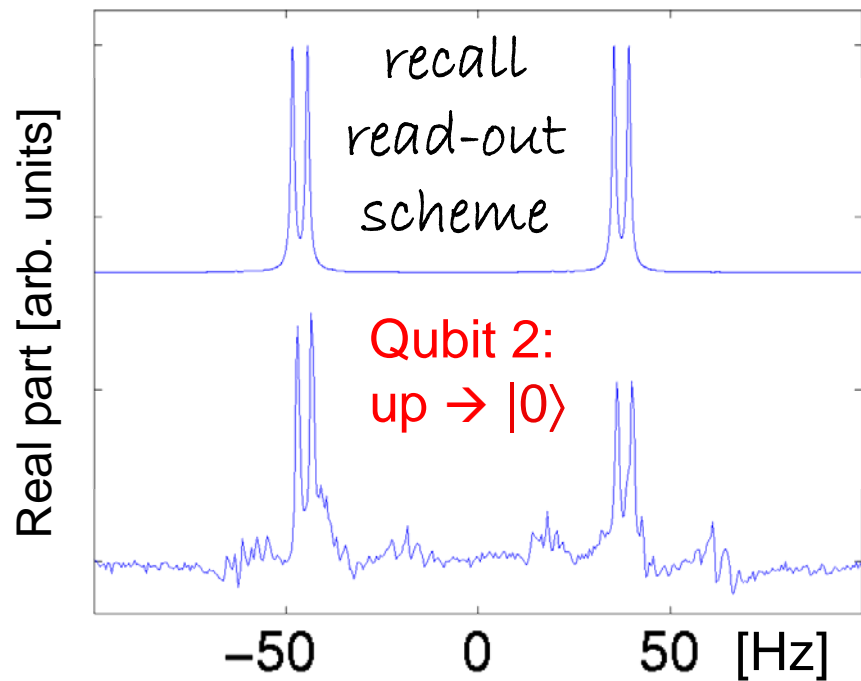
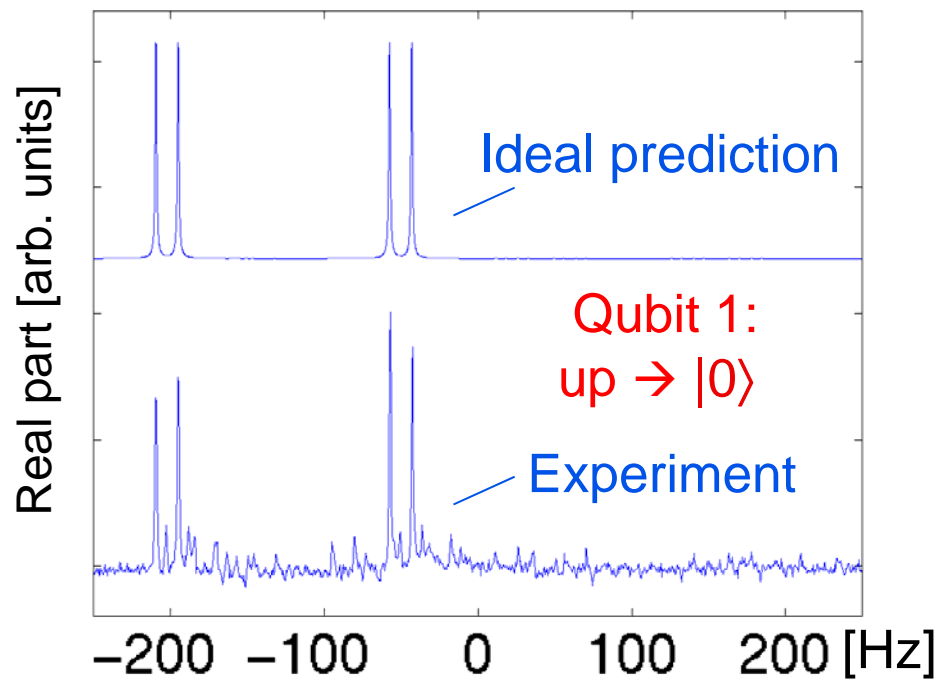


$\pi/2$ X- or Y-rotations (H and gates)

π X-rotations (refocusing)

Z - rotations

> 300 pulses, \approx 720 ms



“Easy” case ^{period 2} ($a=11$)

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$|000\rangle$ 0

$|100\rangle$ 4



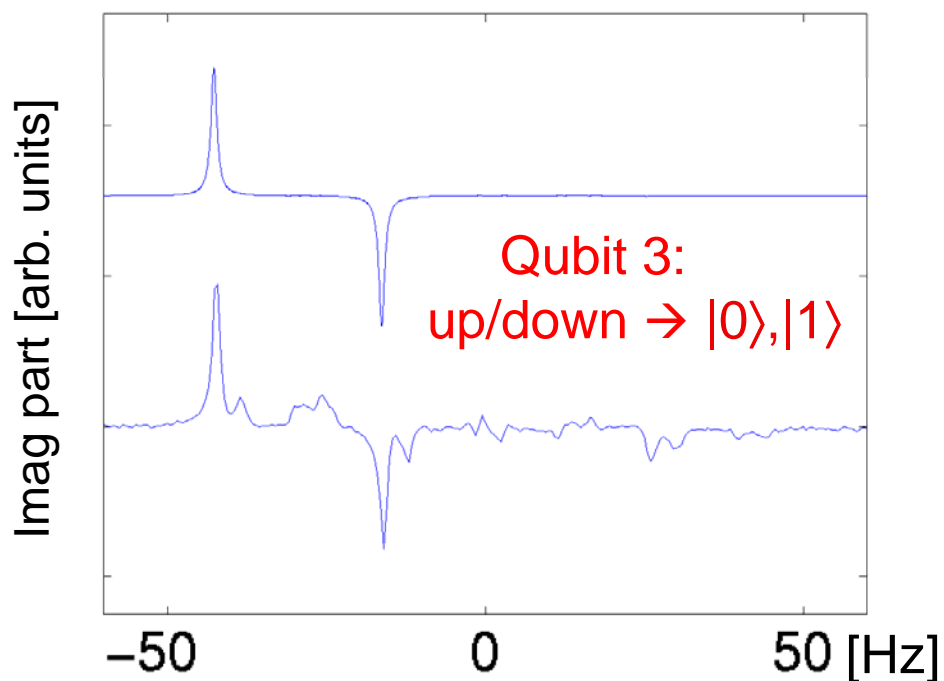
$8 / r = 4$

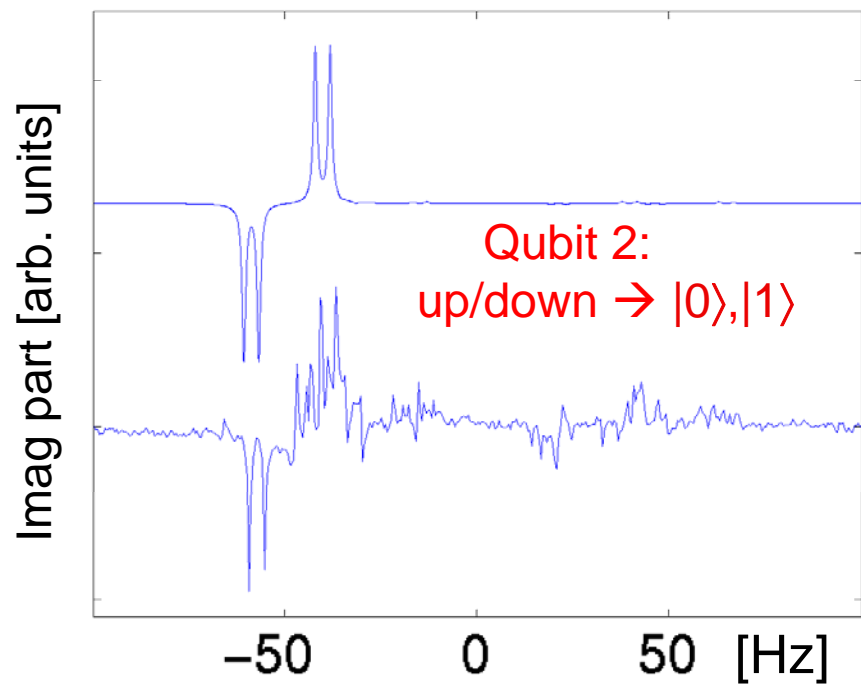
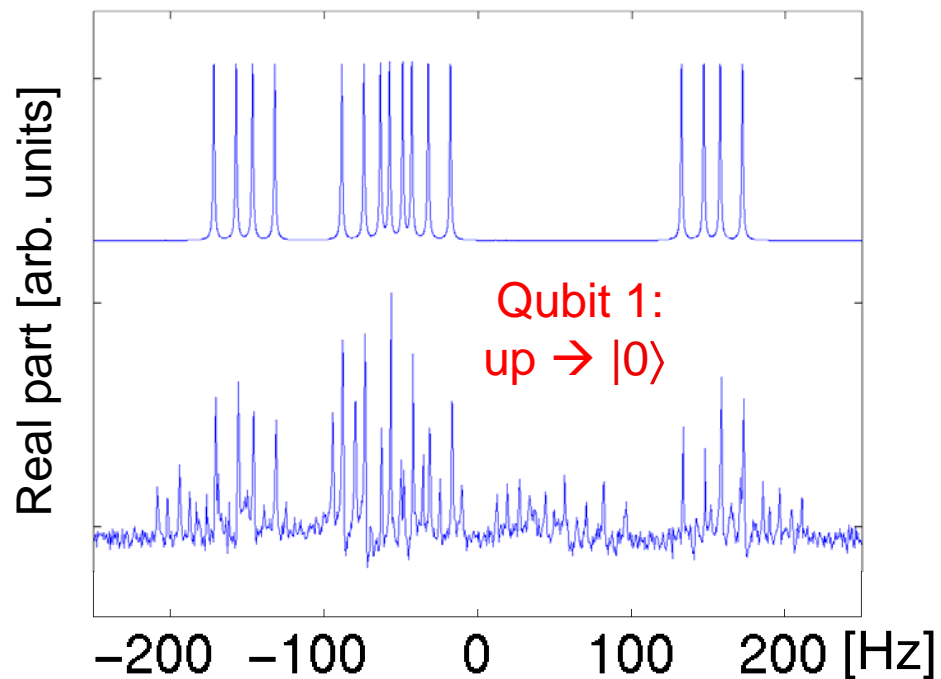
$r = 2$ period

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

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

$$15 = 3 \times 5$$





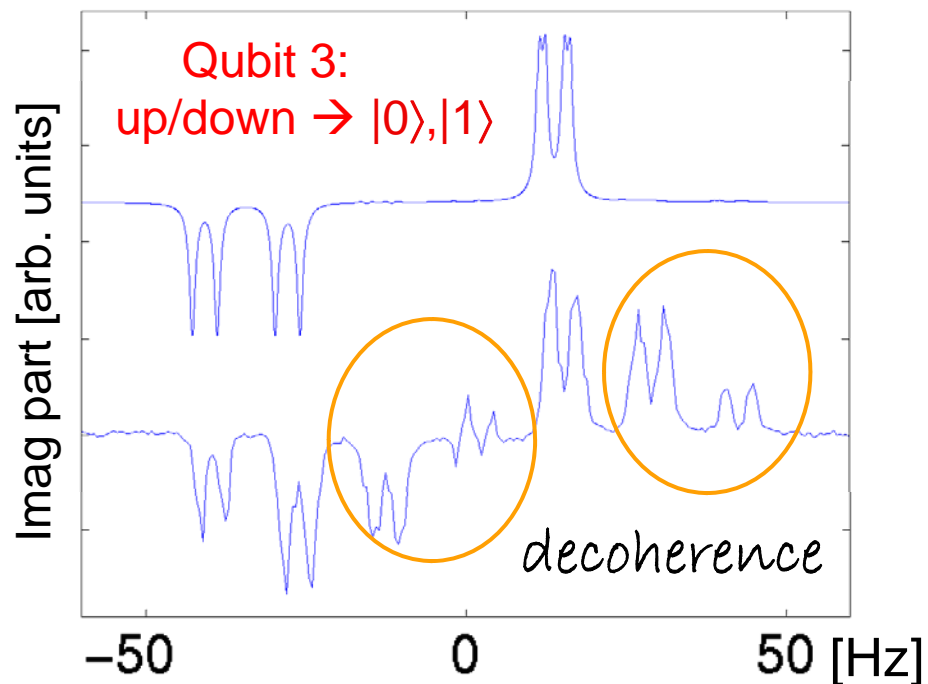
“Hard” case ^{period 4} ($a=7$)

$ 000\rangle$	0		
$ 010\rangle$	2	\rightarrow	$8 / r = 2$
$ 100\rangle$	4		$r = 4$ period
$ 110\rangle$	6		

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

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

$$15 \cong 3 \times 5$$



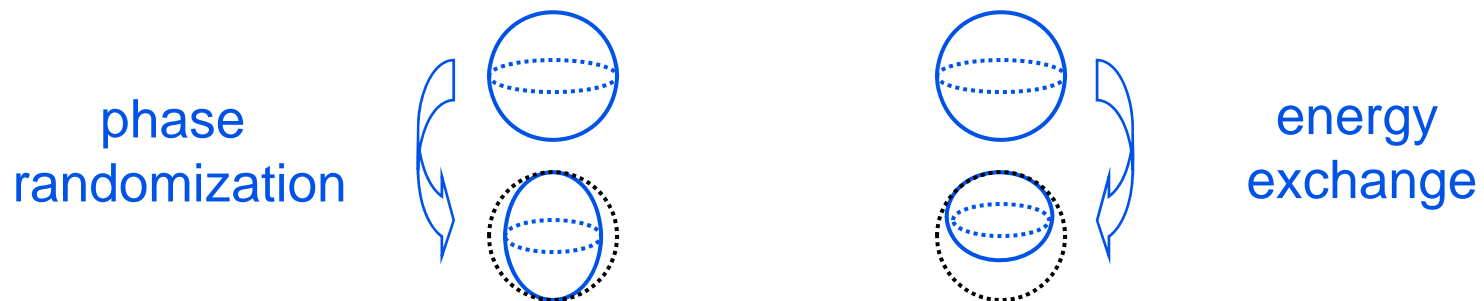
Model quantum noise (decoherence)

Spins interact with the environment

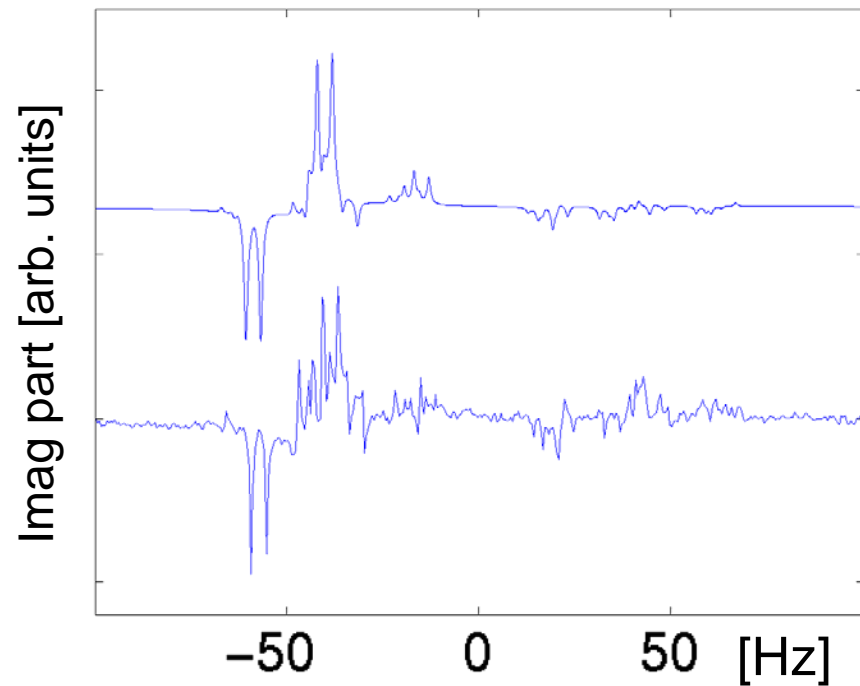
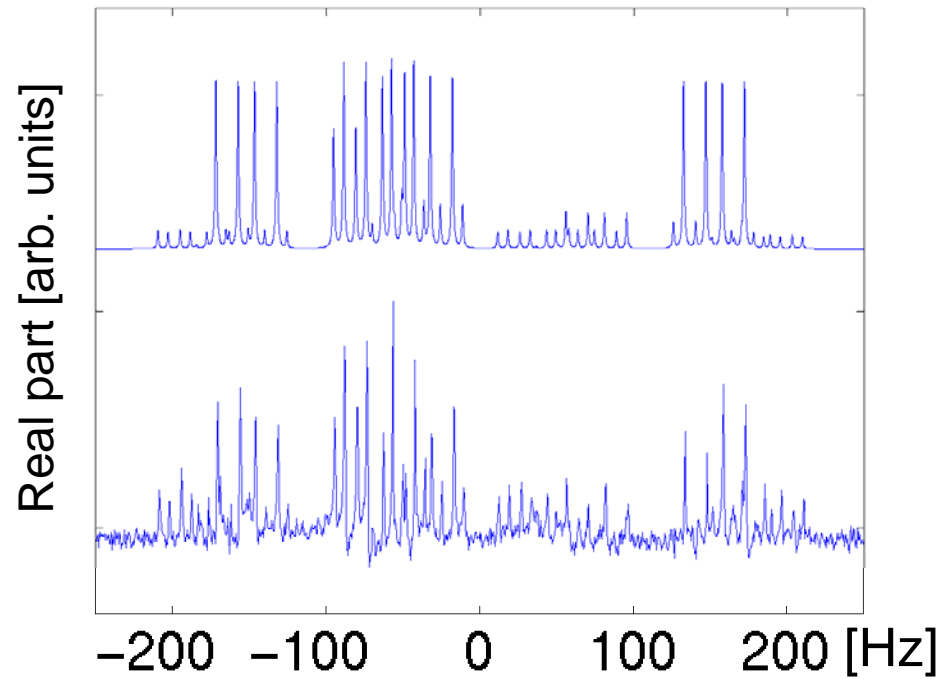


Decoherence

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



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

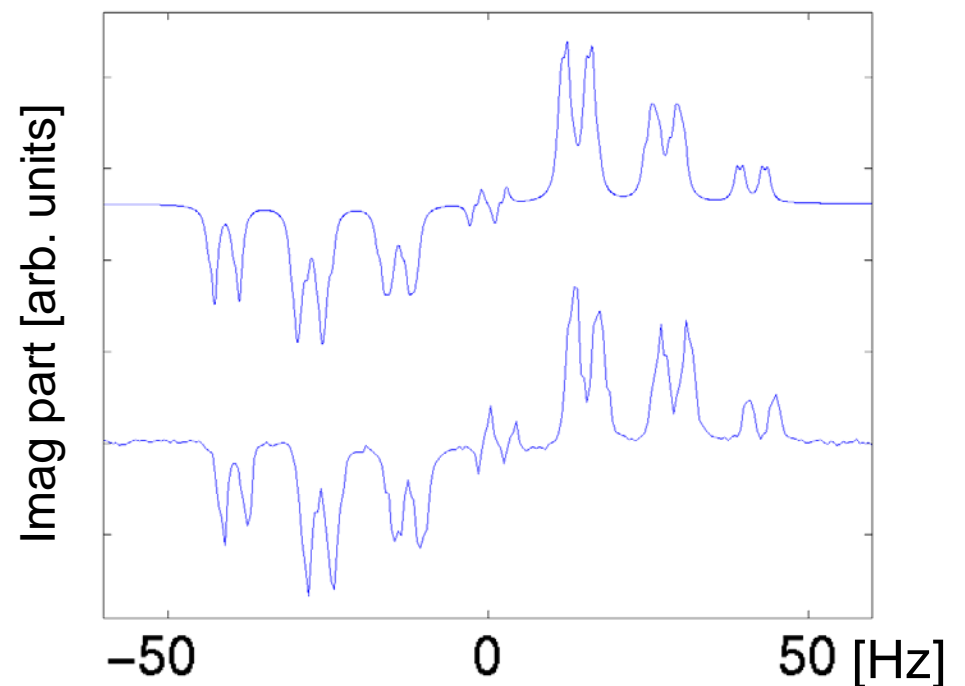


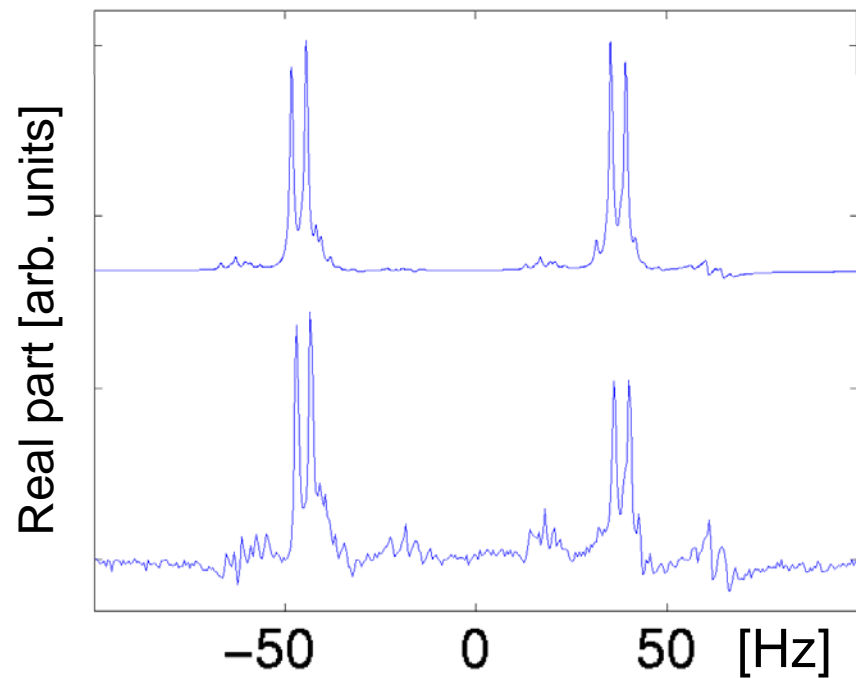
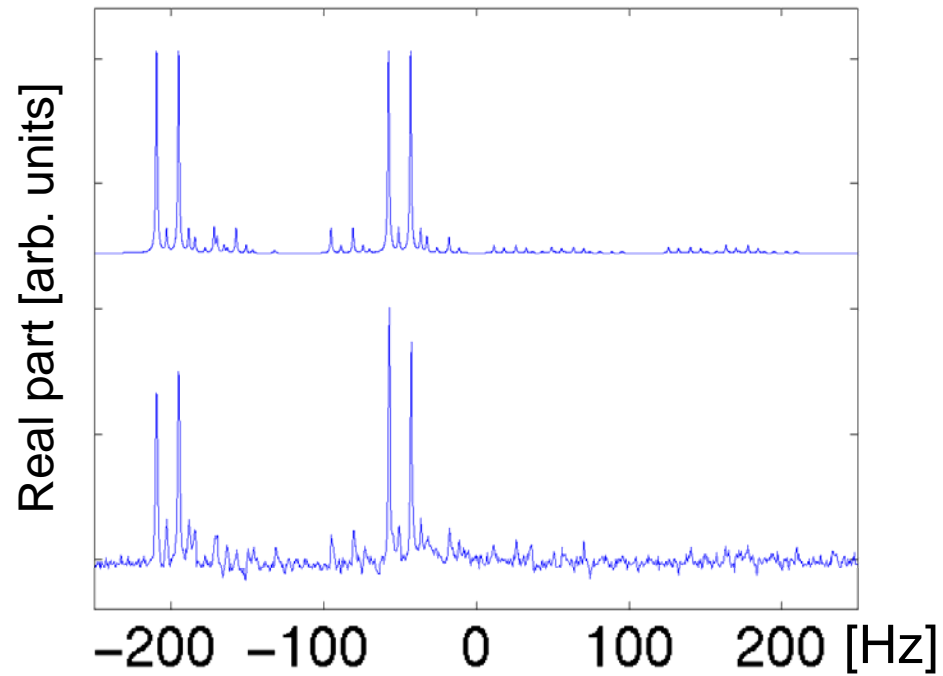
Simulation of decoherence (1)

fundamental limit

hard case

decoherence can be understood and modeled





Simulation of decoherence (2)

fundamental limit

easy case

decoherence can be understood and modeled

