Lecture 10, May 06, 2017

This week:

- Quantum Computing with liquid-state NMR
  - Nuclear Spins ins Molecules
  - Nuclear Spin control
    - Initialization
    - Read-Out
    - Single & Multi Qubit gates

Introductory Review Articles:

- L. M. K. Vandersypen & I. L. Chuang, NMR techniques for quantum control and computation, *RMP* **76**, (2004)
- N. A. Gershenfeld, Isaac L. Chuang, Bulk spin-resonance quatum computation, *Science* **275**, 350 (1997)

Please take a seat
in the front center part of the lecture hall
if you do not mind.

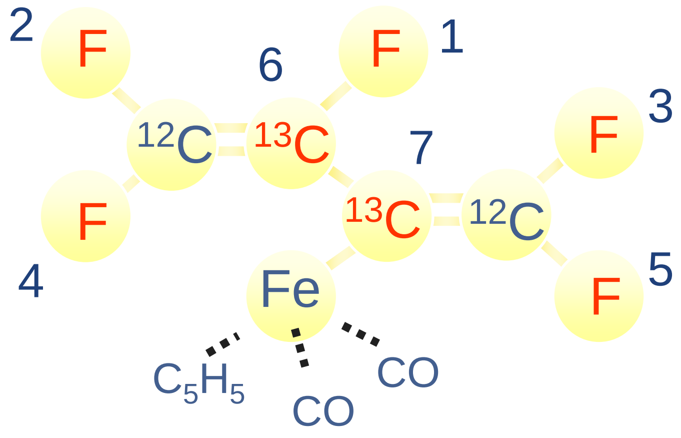
NMR Quantum Computing

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

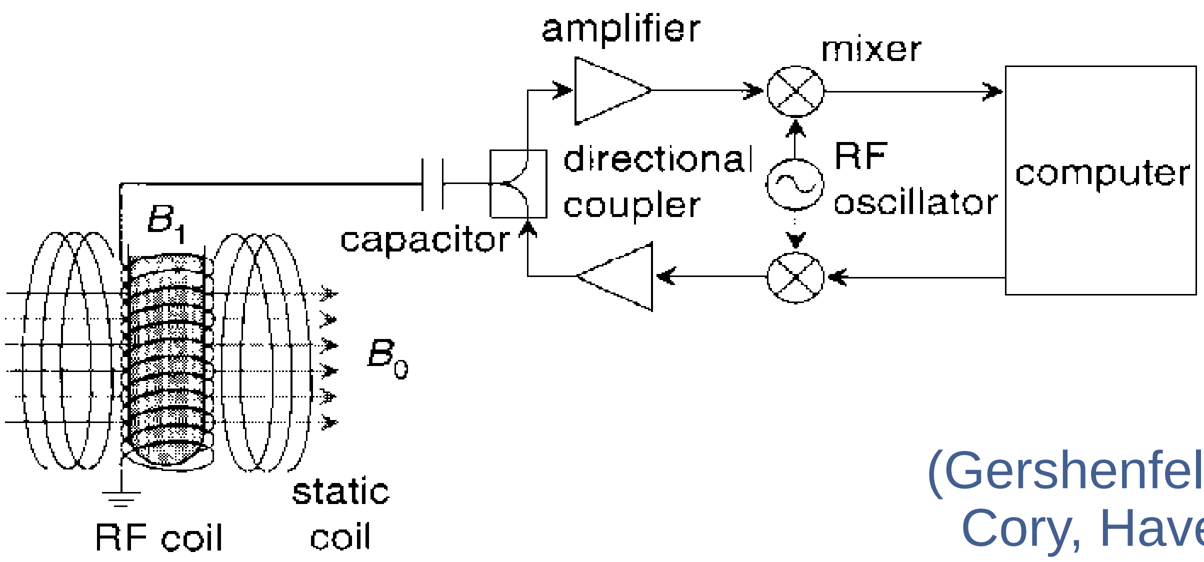
Goals of this lecture

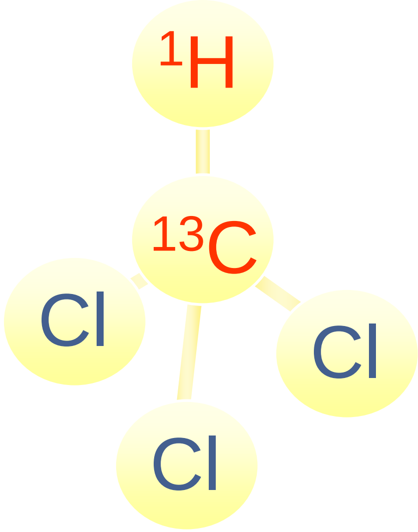
Survey of NMR quantum computing

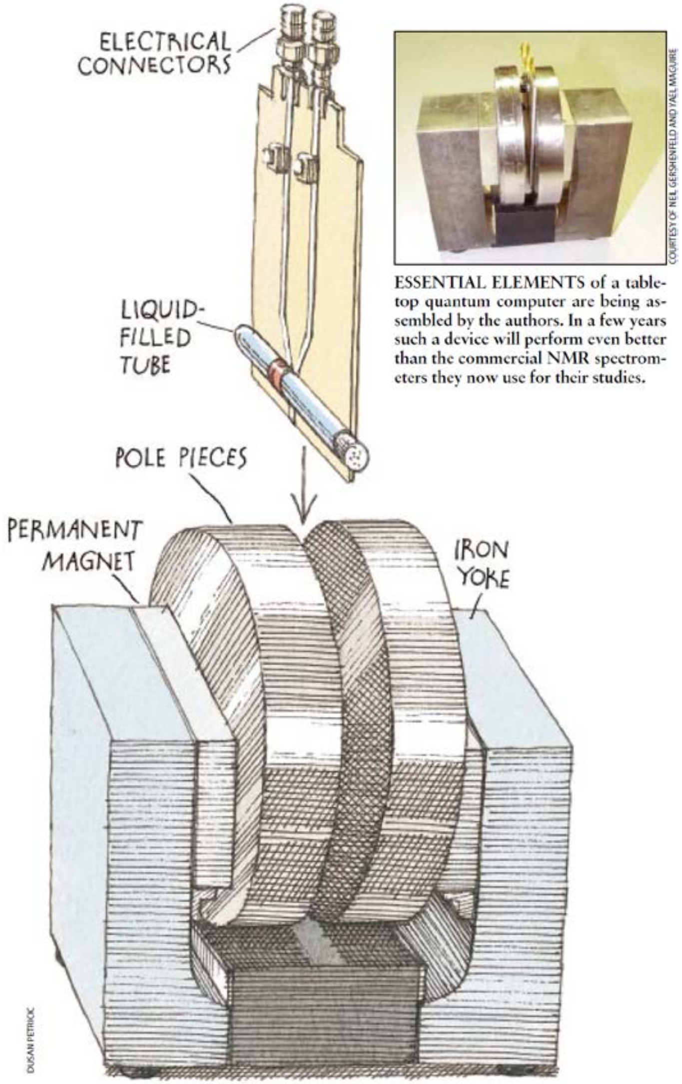
- Principles of NMR QC
- Techniques for qubit control
- State of the art
- Future of spins for QIPC
- Example: factoring 15

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





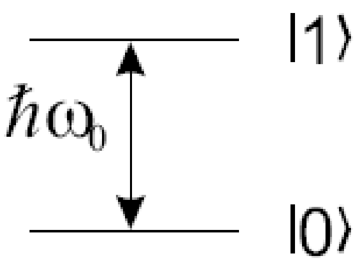


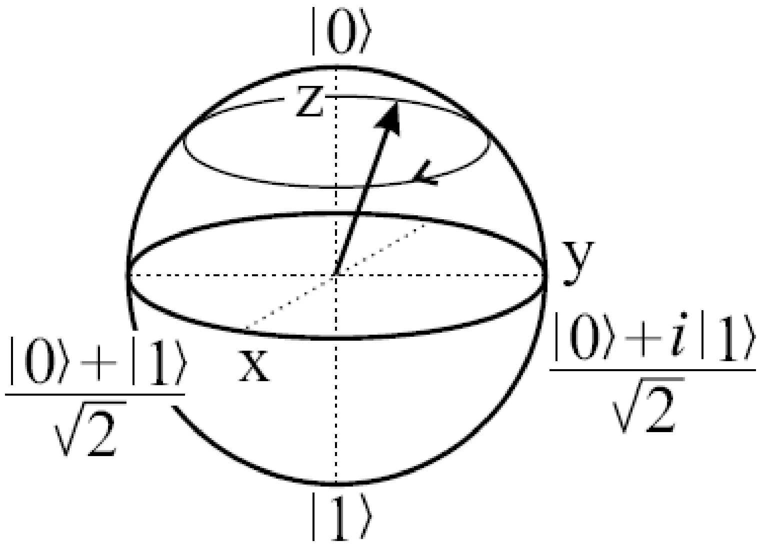
ESSENTIAL ELEMENTS of a tabletop quantum computer are being assembled by the authors. In a few years such a device will perform even better than the commercial NMR spectrometers they now use for their studies.

(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: $\vec{M} = \gamma \hbar \vec{I}$

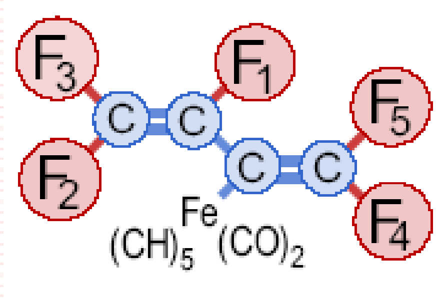
energy: $H_0 = -\vec{M} \cdot \vec{B}_0$

gyromagnetic (g-)factor: γ

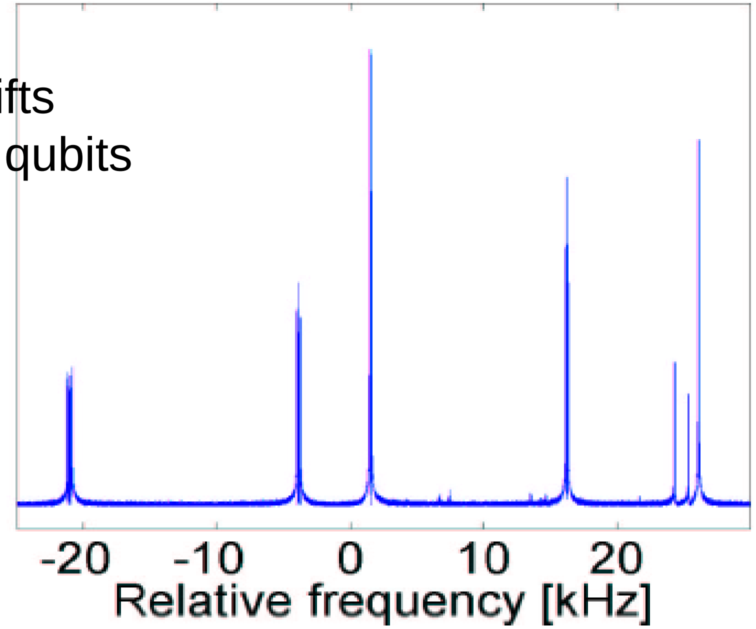
Nuclear spin Hamiltonian
Multiple spins

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

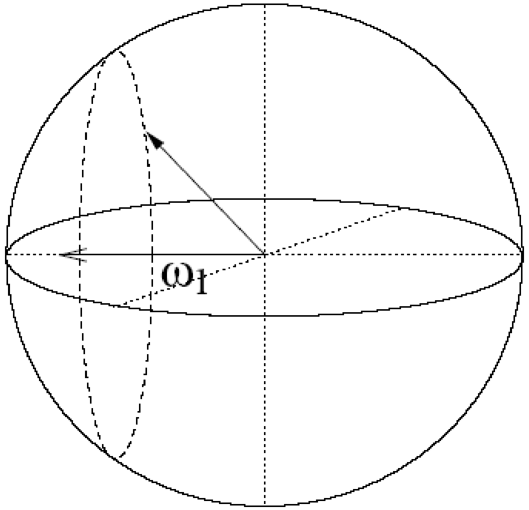
$$\mathcal{H} = -\hbar\,\omega_0 \underbrace{I_z}_{\sigma_z} - \hbar\omega_1 \left[\cos(\omega_{rf}t+\phi)\underbrace{I_x}_{\sigma_x} + \sin(\omega_{rf}t+\phi)\underbrace{I_y}_{\sigma_y}\right]$$

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

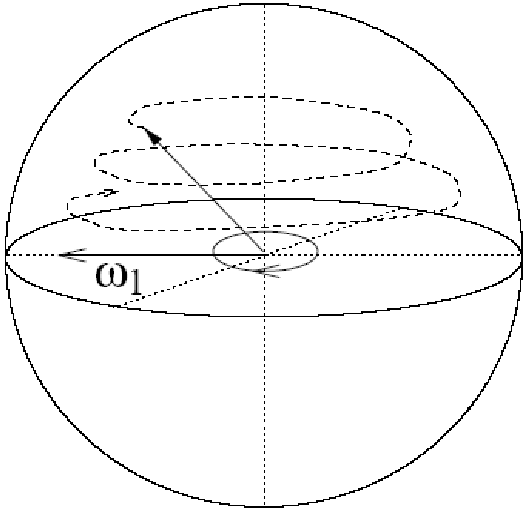
$$\mathcal{H}^{rot} = -\hbar\,(\omega_0 - \omega_{rf})\; I_z - \hbar\omega_1 \left[\cos\phi\, I_x + \sin\phi\, I_y\right]$$

rotating wave approximation

typical strength I_x, I_y : up to 100 kHz



Rotating frame



Lab frame

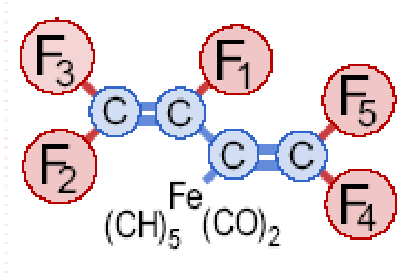
Nuclear spin Hamiltonian
Coupled spins

J>0: antiferro mag.

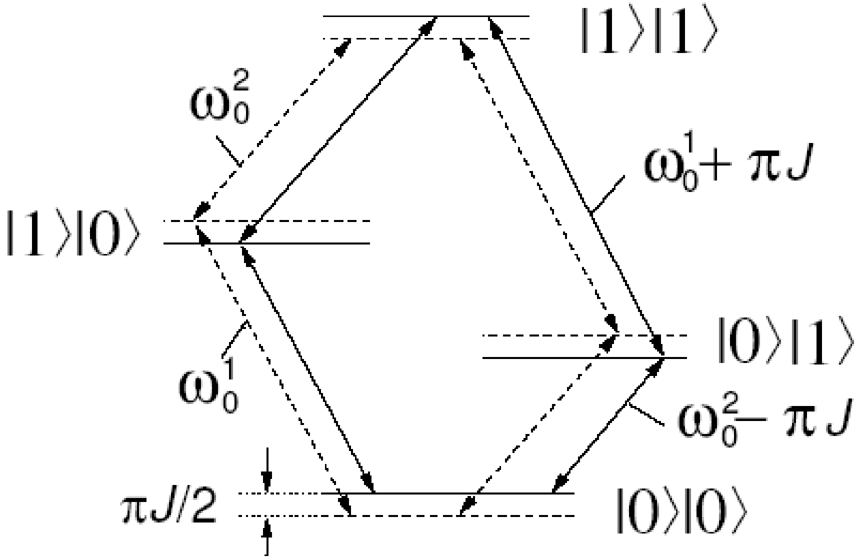
J<0: ferro-mag.

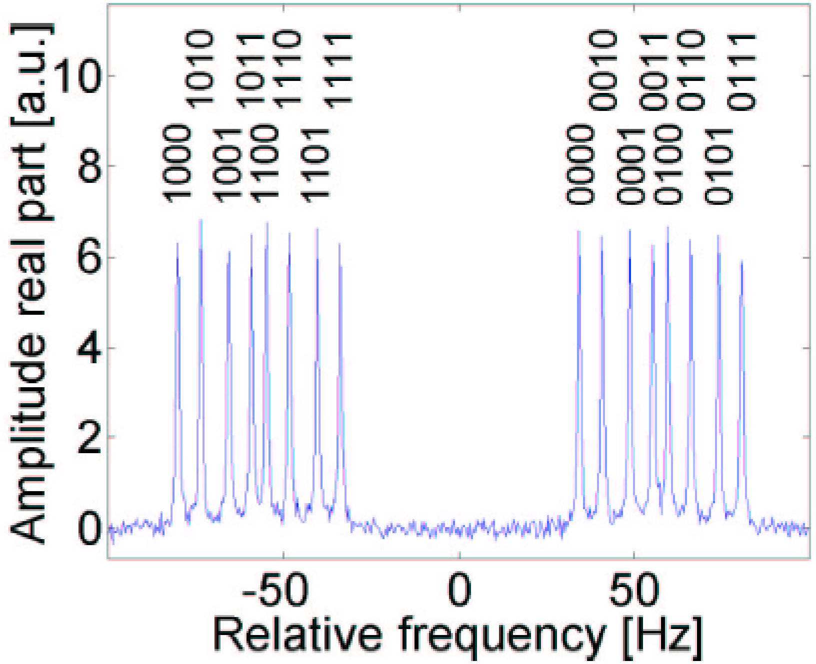
$$\mathcal{H}_J = \hbar \sum_{i<j}^{n} 2\pi J_{ij} I_z^i I_z^j$$

Typical values: *J* up to few 100 Hz



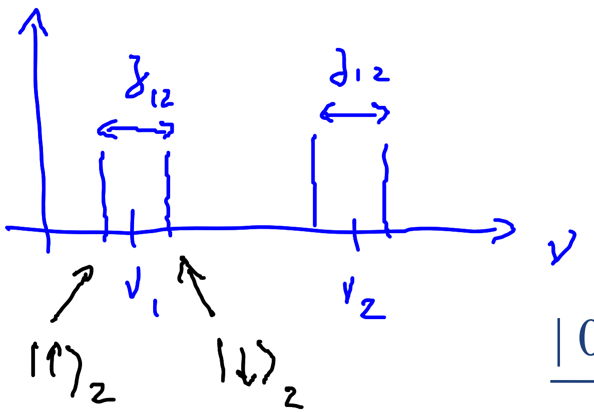
16 configurations

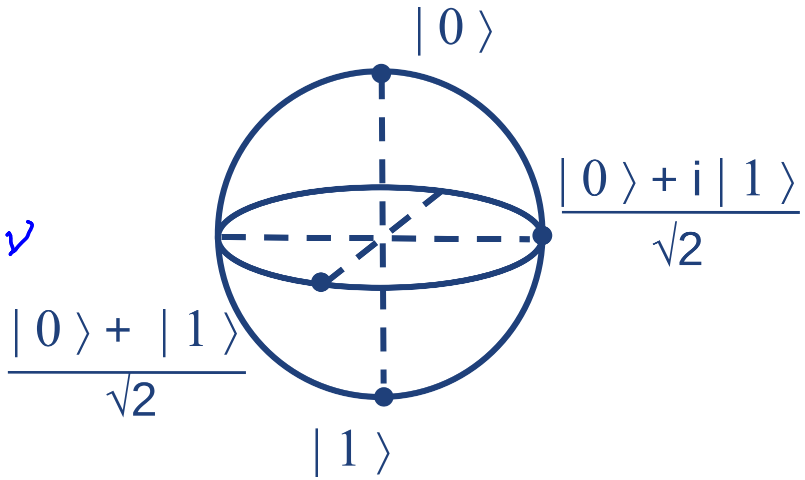


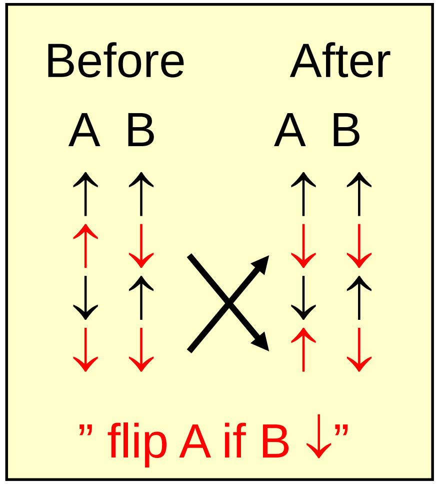


solid (dashed) lines are (un)coupled levels

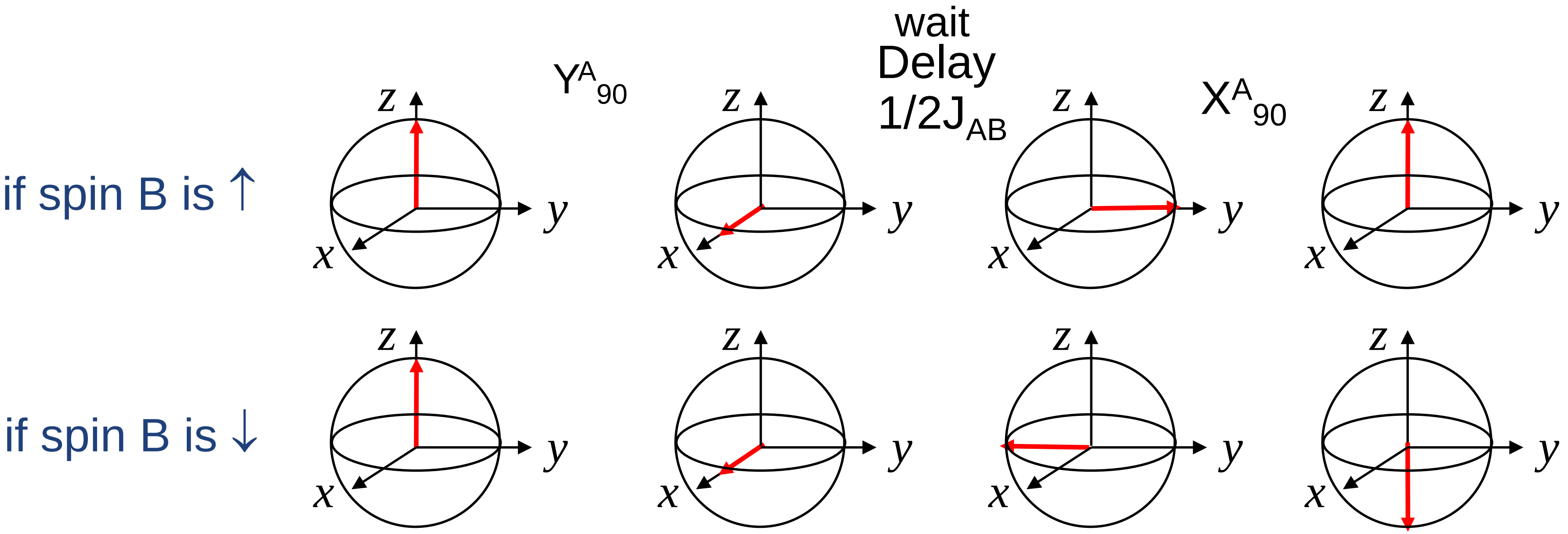
Controlled-NOT in NMR







A target bit
B control bit

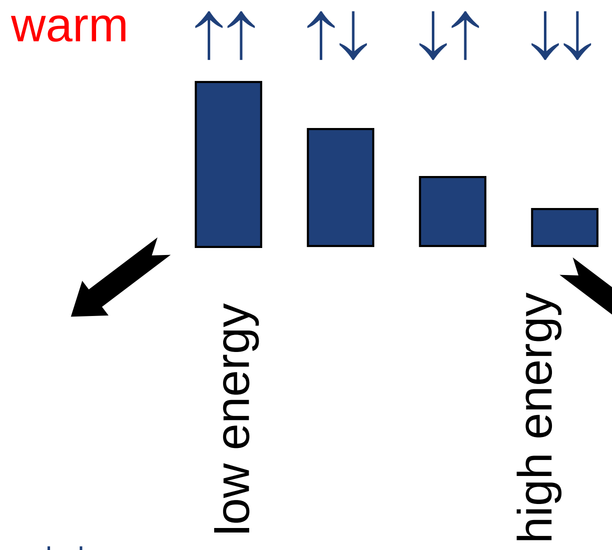


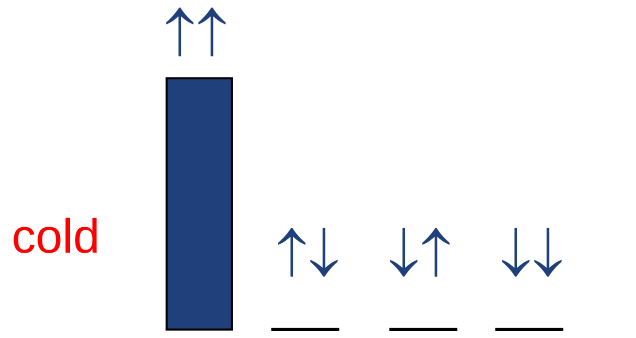
different rotation direction depending on control bit

time

Making room temperature spins look cold

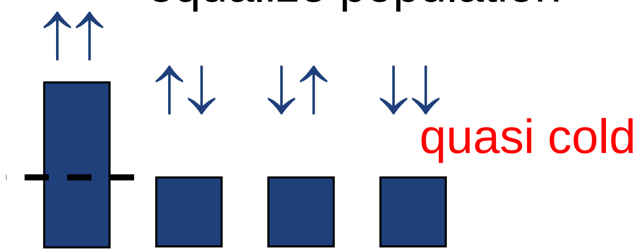
- (Cool to mK)
- Optical pumping
- DNP, …



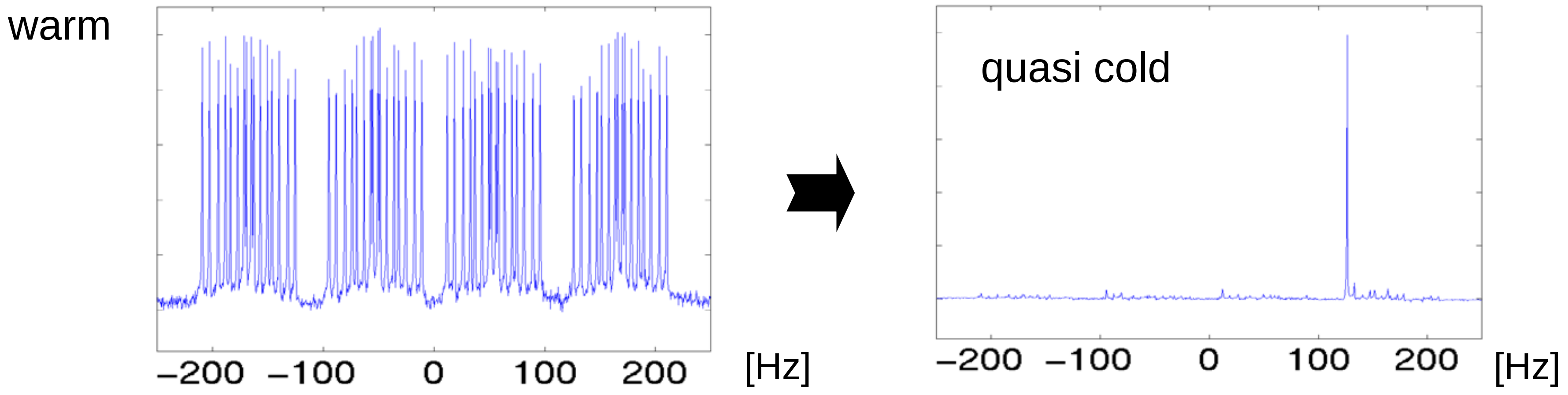


Effective pure state
(Gershenfeld&Chuang, Science ‘97,
Cory, Havel & Fahmi, PNAS ‘97)

equalize population

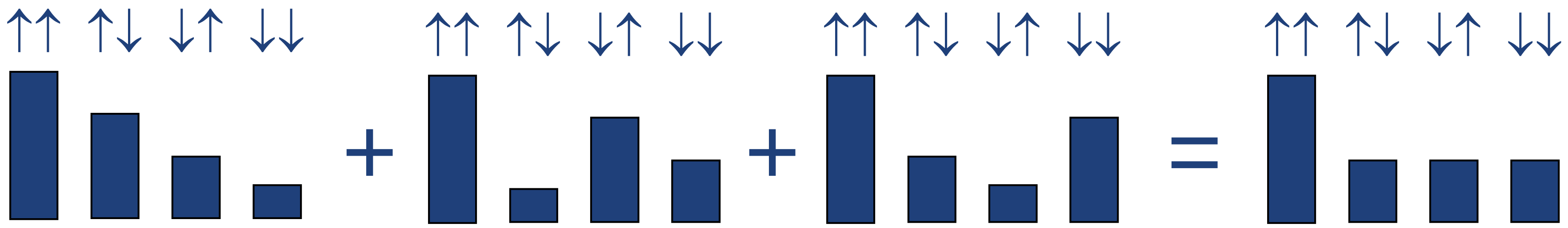


Look exactly like cold spins !



Effective pure state preparation

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



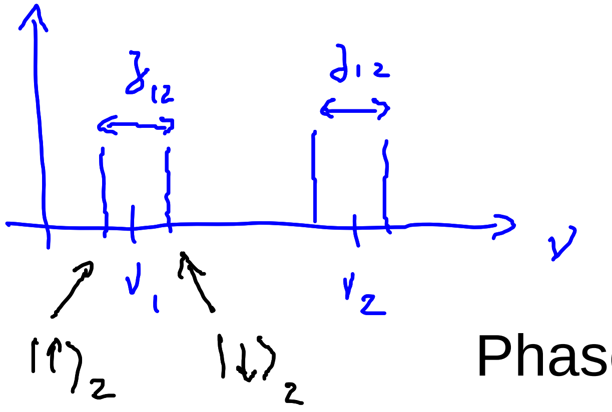
Later ≈ (2^N - 1) / N experiments (Vandersypen *et al.*, PRL 2000)

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

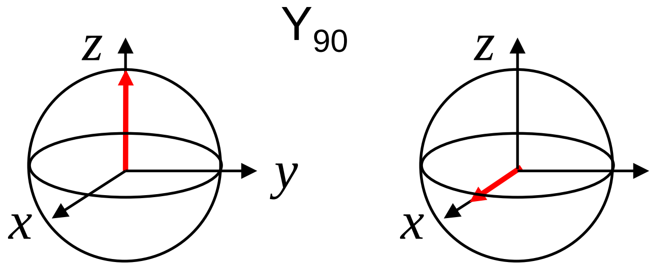
(2) Work in subspace (Gershenfeld&Chuang, Science 1997)

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

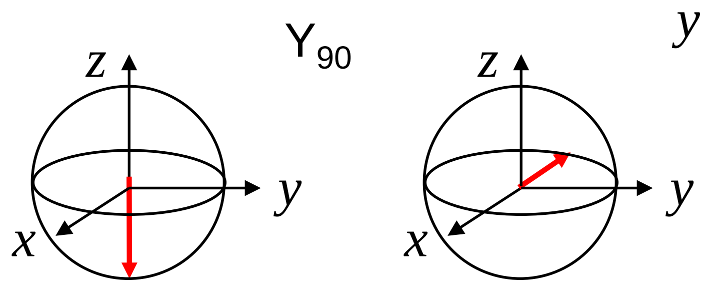
Read-out in NMR



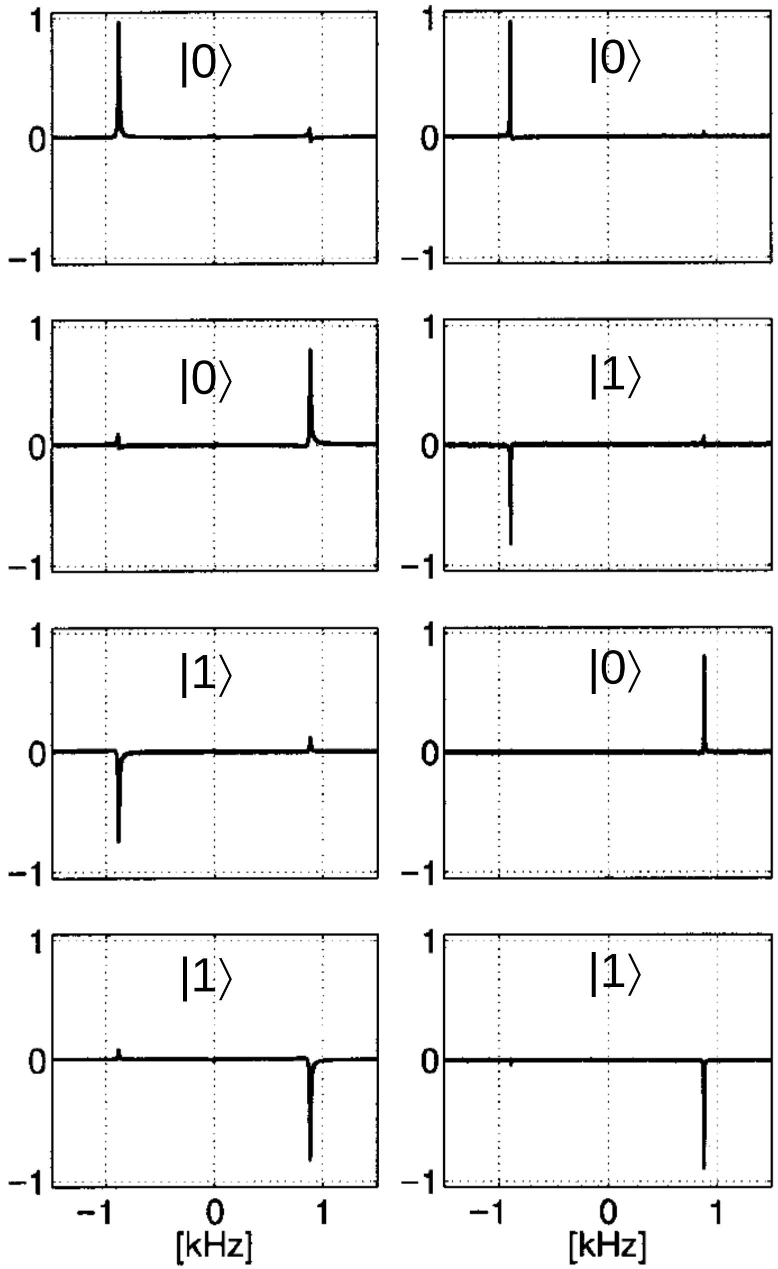
Phase sensitive detection



positive signal for |0> (in phase)



negative signal for |1> (out of phase)



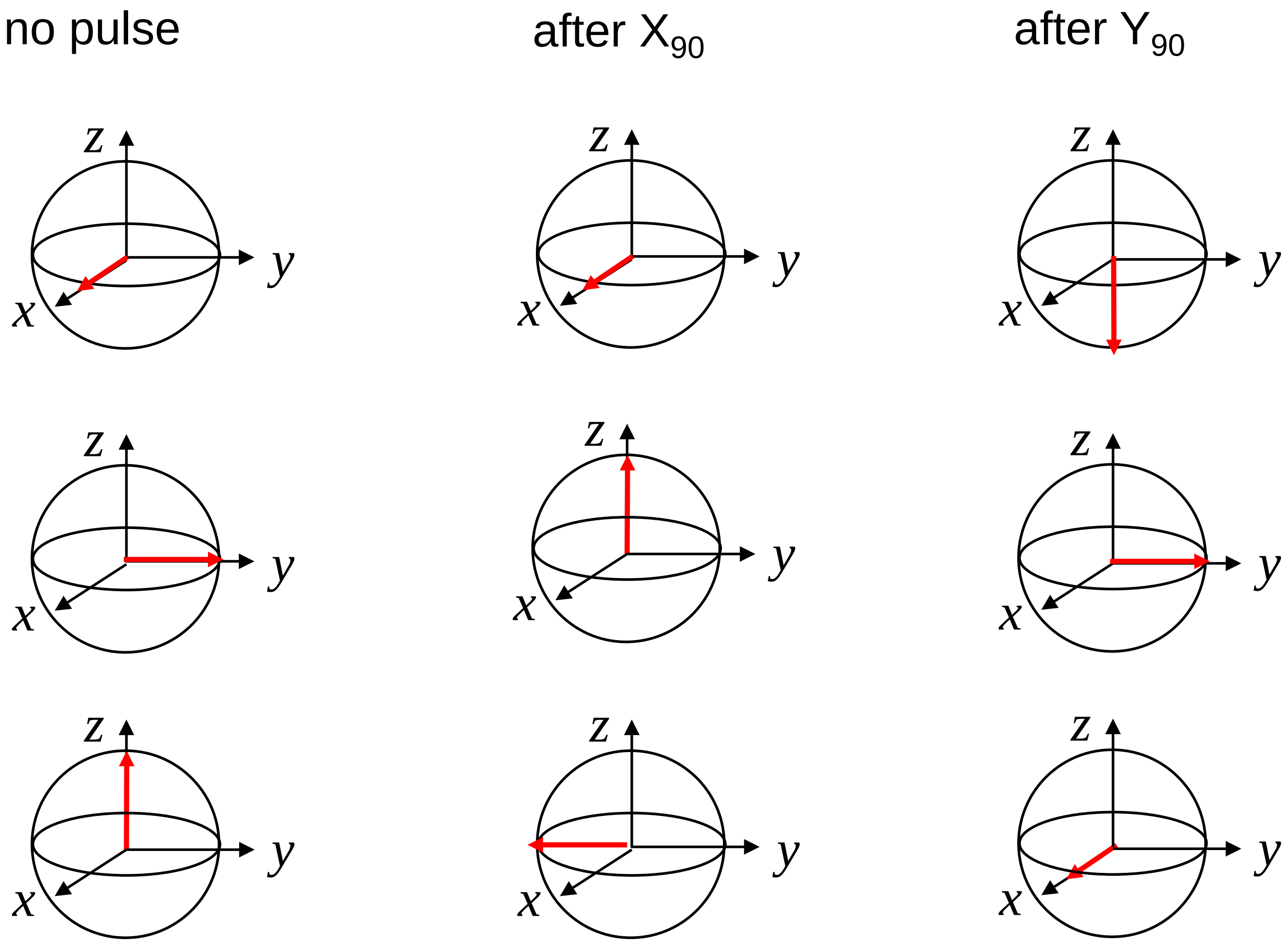
Measurements of single systems versus ensemble measurements

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



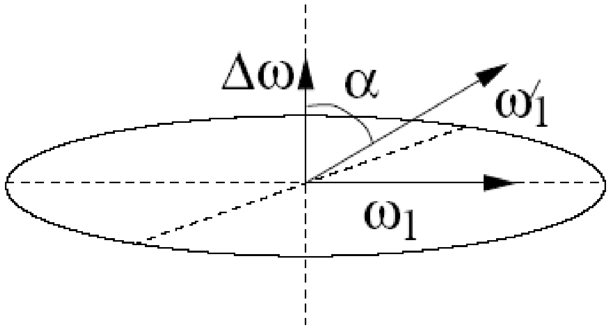
Outline

Survey of NMR quantum computing

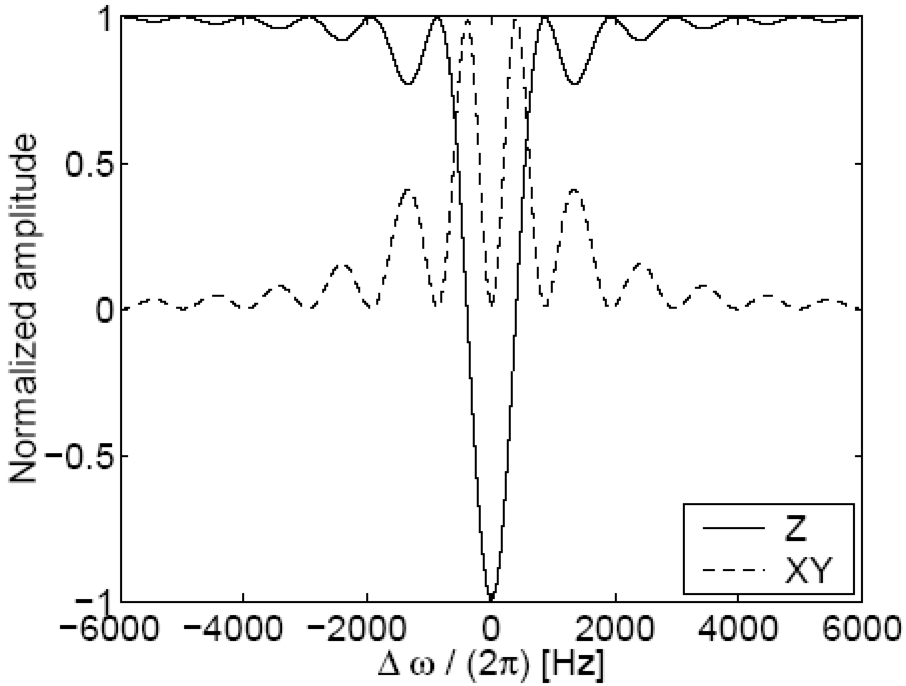
- Principles of NMR QC
- Techniques for qubit control
- Example: factoring 15
- State of the art
- Outlook

Off-resonance pulses and spin-selectivity

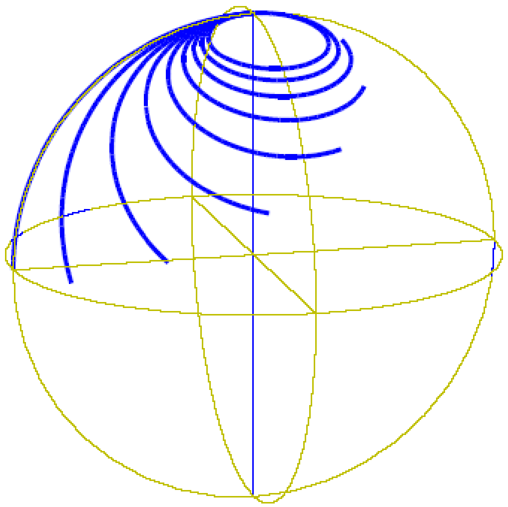
$$\mathcal{H}^{rot} = -\hbar\,(\omega_0 - \omega_{rf})\; I_z - \hbar\omega_1 \left[\cos\phi\, I_x + \sin\phi\, I_y\right]$$



spectral content of a square pulse

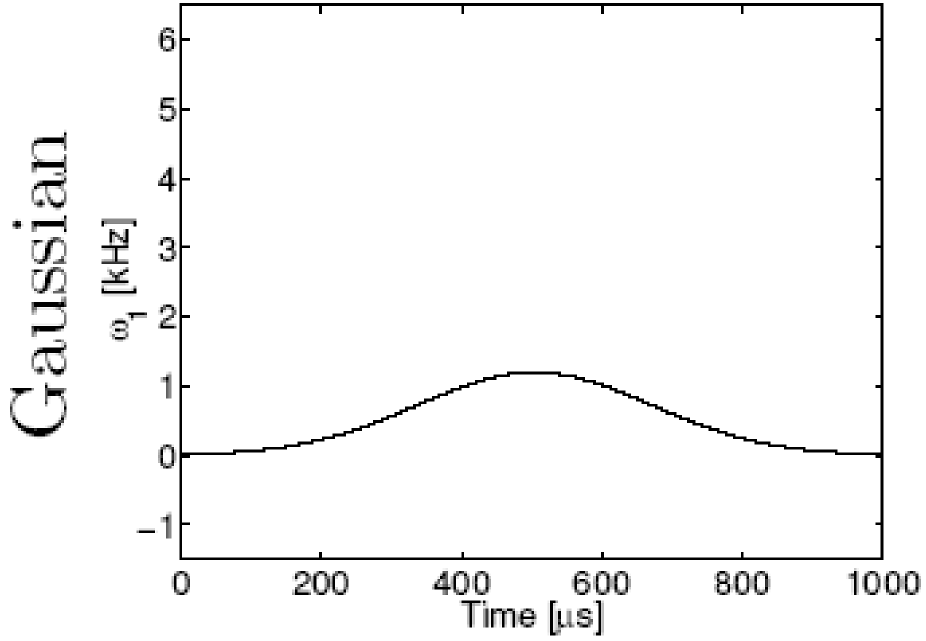


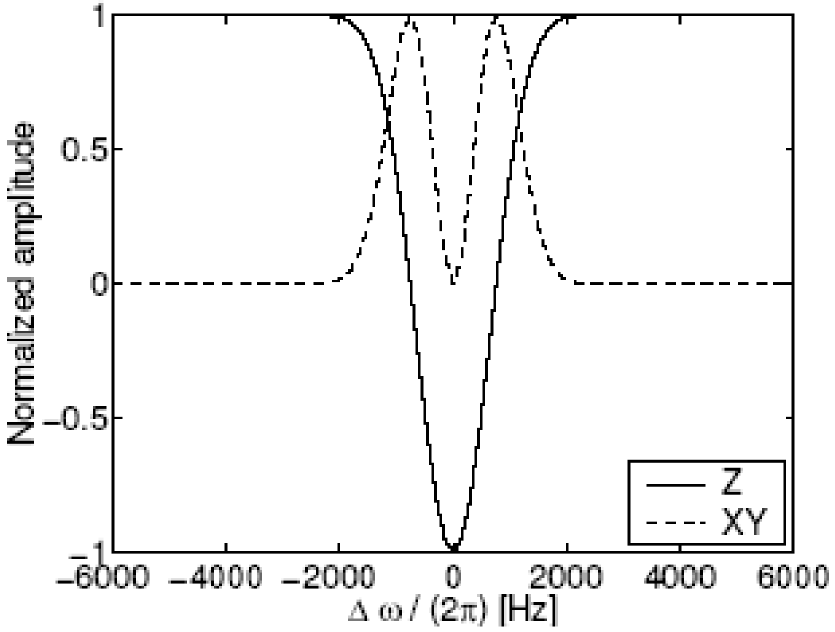
off-resonant pulses induce eff. σ_z rotation in addition to $\sigma_{x,y}$



may induce transitions in other qubits

Pulse shaping for improved spin-selectivity





less cross-talk

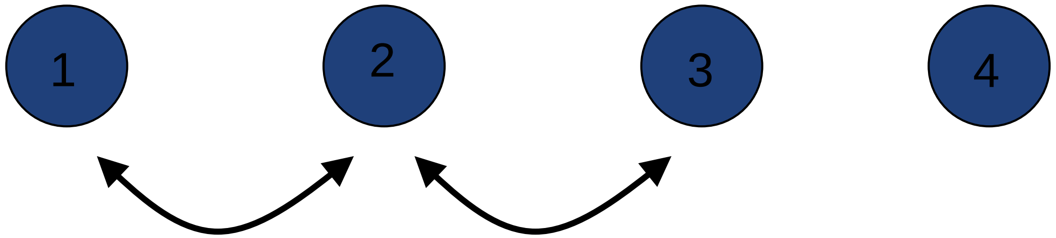
Missing coupling terms: Swap

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

Missing couplings: swap states along qubit network

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

as discussed
in exercise class

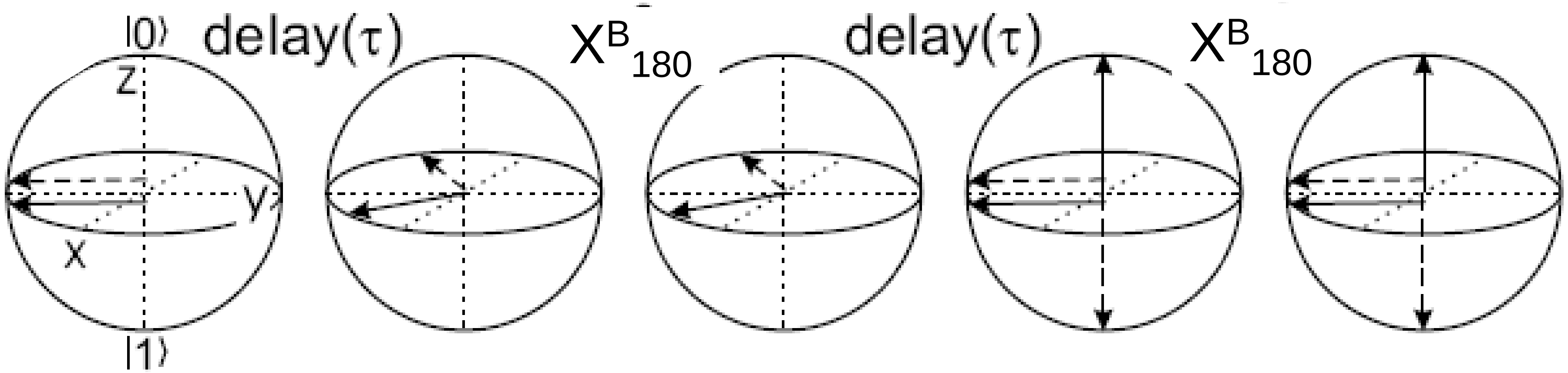


“only” a linear overhead ...

Undesired couplings: refocus

opt. 1: act on qubit B

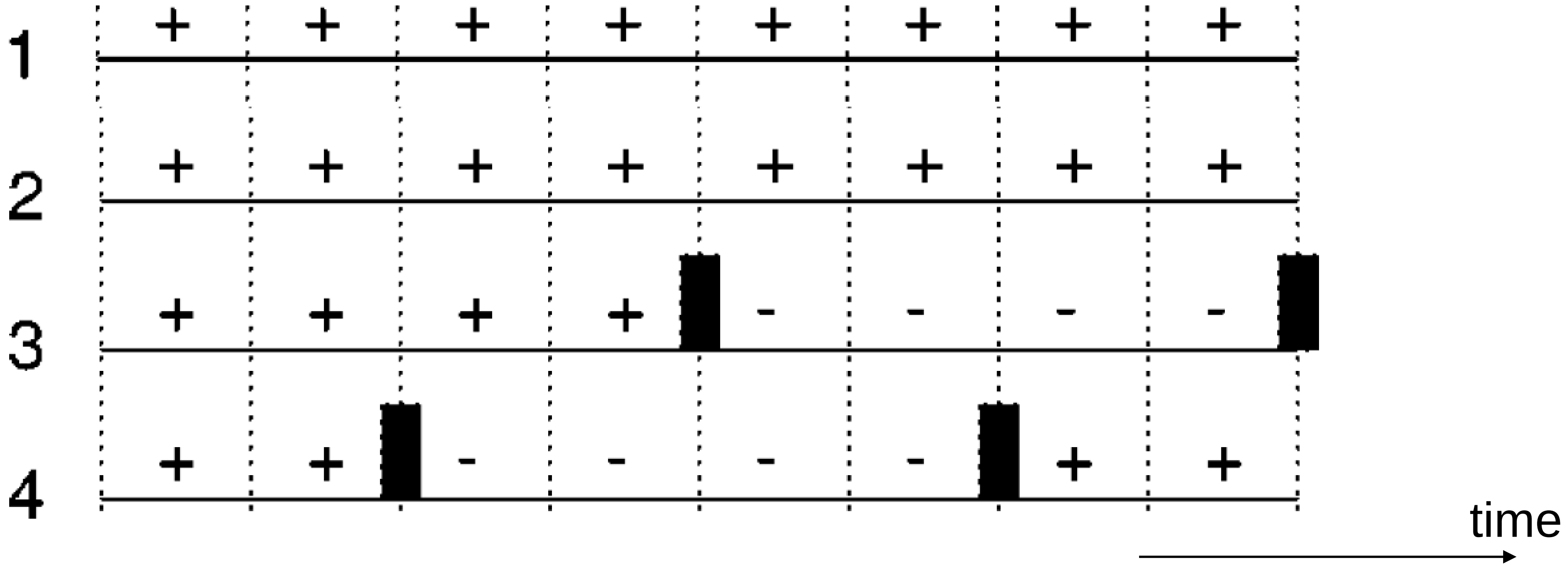
remove effect of coupling *during delay times*



opt. 2: act on qubit A

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

Undesired couplings: refocus



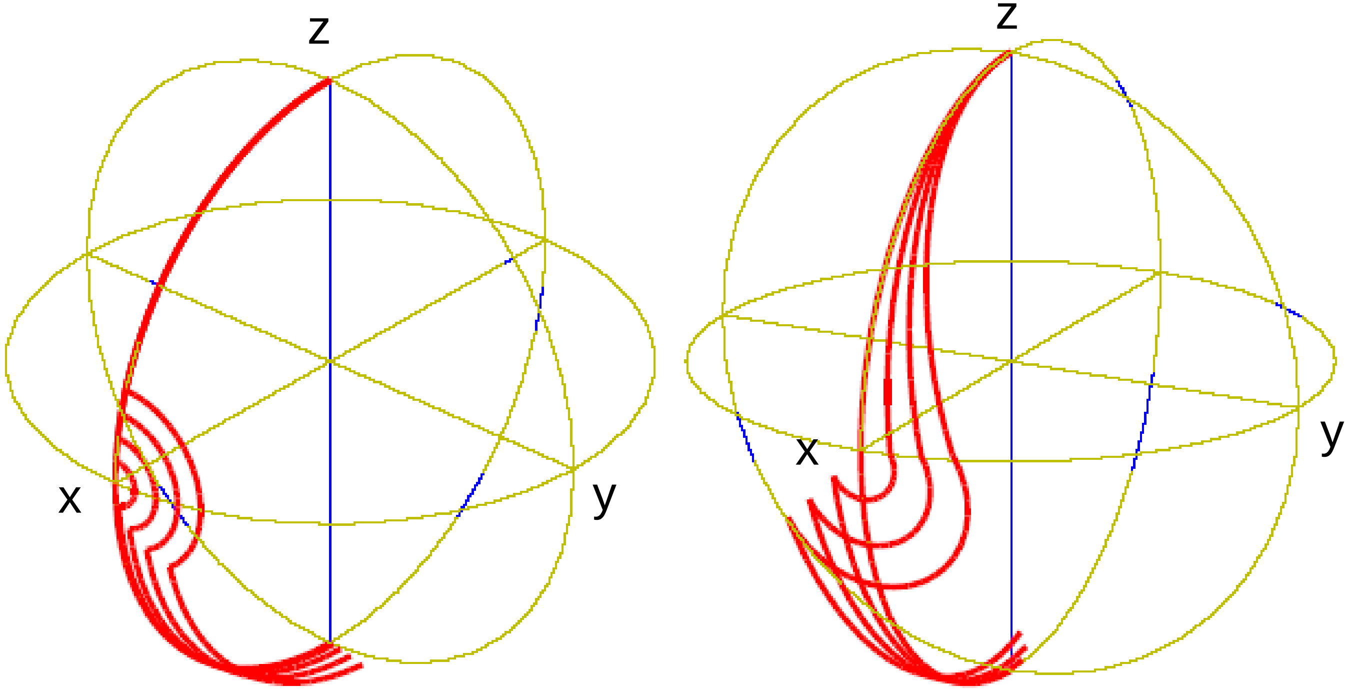
-> no net coupling between qubits 2 - 4
-> Effective coupling only between qubit 1 and 2

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)

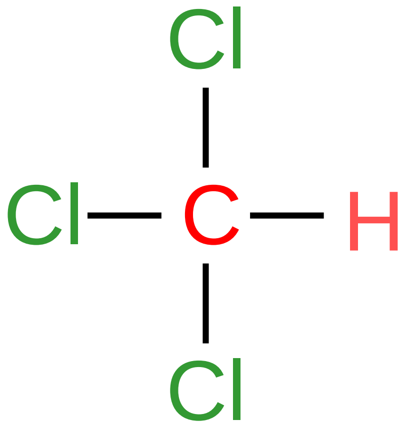
- stable, available, soluble, ...

required to make spins of same type addressable

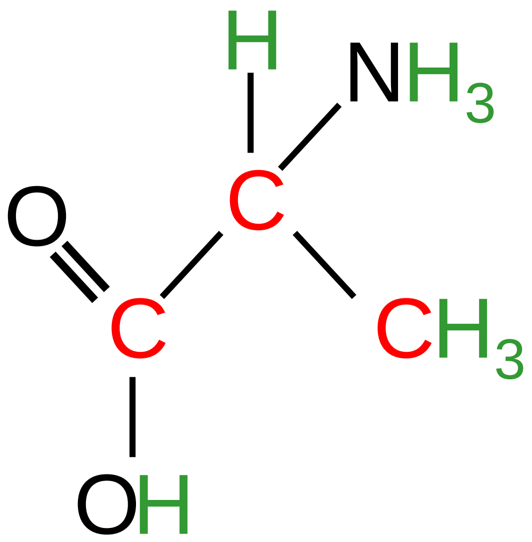
Quantum computer molecules (1)

red nuclei are used as qubits:

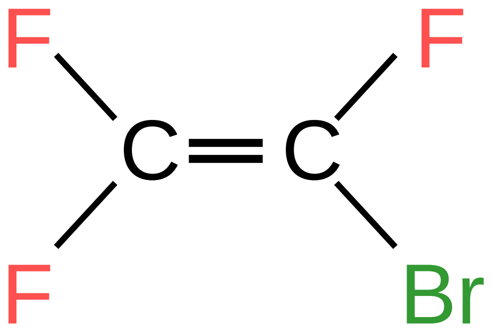
Grover / Deutsch-Jozsa



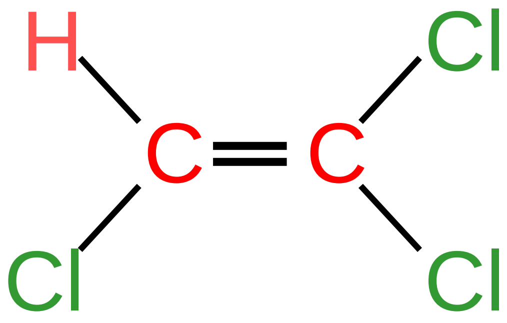
Q. Error correction



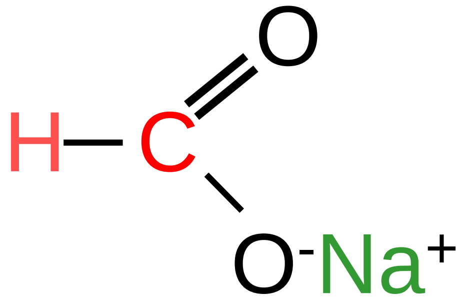
Logical labeling / Grover



Teleportation

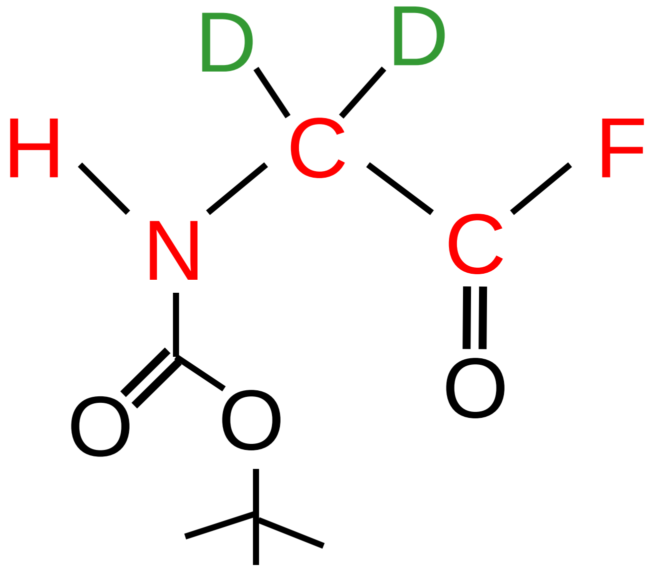


Q. Error Detection

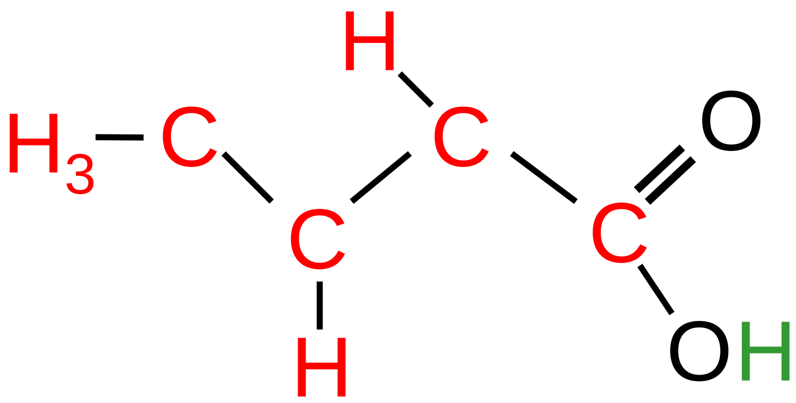


Quantum computer molecules (2)

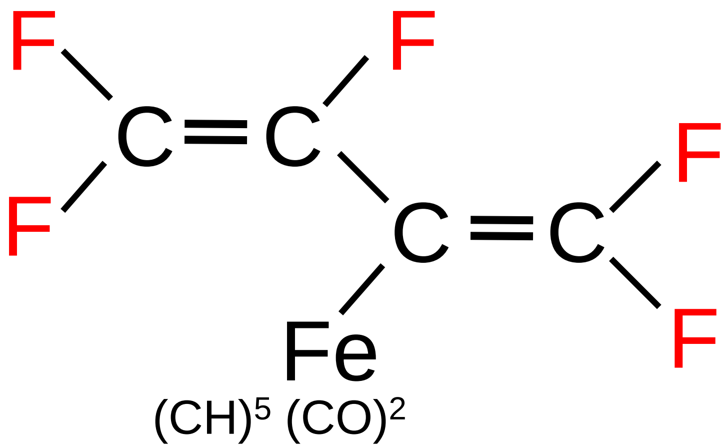
Deutsch-Jozsa



7-spin coherence



Order-finding



Outline

Survey of NMR quantum computing

- 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 ~ 1 / 2^n [at least in practice]
- Coherence time typically goes down with molecule size
- We have not yet reached the accuracy threshold ...
- Ensemble averaged measurement <-> error correction

Main sources of errors in NMR QC

Early on (heteronuclear molecules)

inhomogeneity RF field

Later (homonuclear molecules)

*J c*oupling during RF pulses

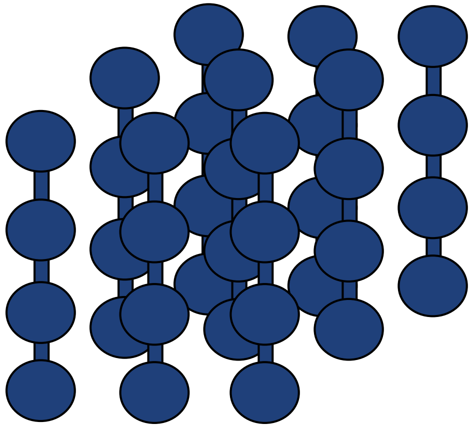
Finally

decoherence

Solid-state NMR ?

molecules in
solid matrix

Cory et al

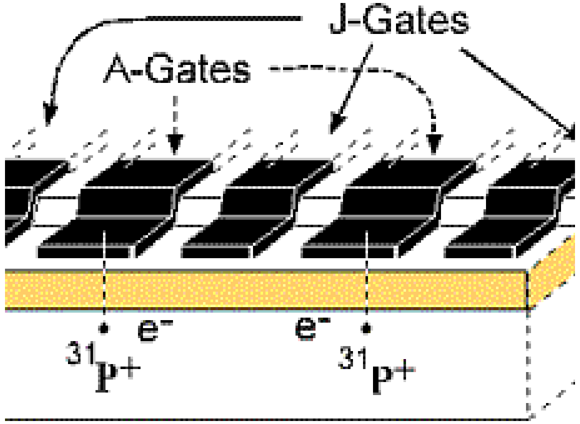


Yamaguchi & Yamamoto, 2000

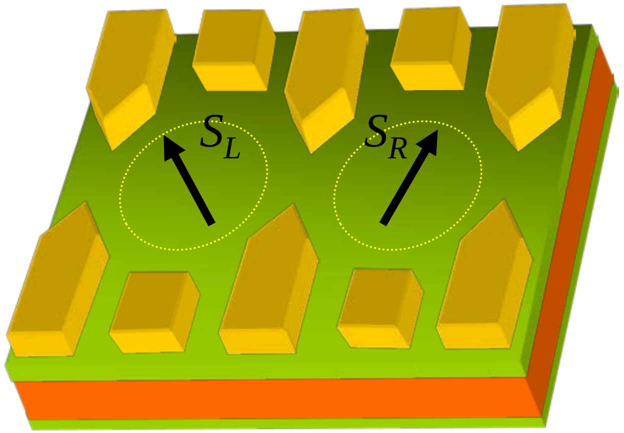
$$\mathcal{H}_J = \hbar \sum_{i<j} 2\pi J_{ij} \vec{I}^i \cdot \vec{I}^j = \hbar \sum_{i<j} 2\pi J_{ij} (I_x^i I_x^j + I_y^i I_y^j + I_z^i I_z^j)$$

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

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.

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

composite number

coprime with N

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

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

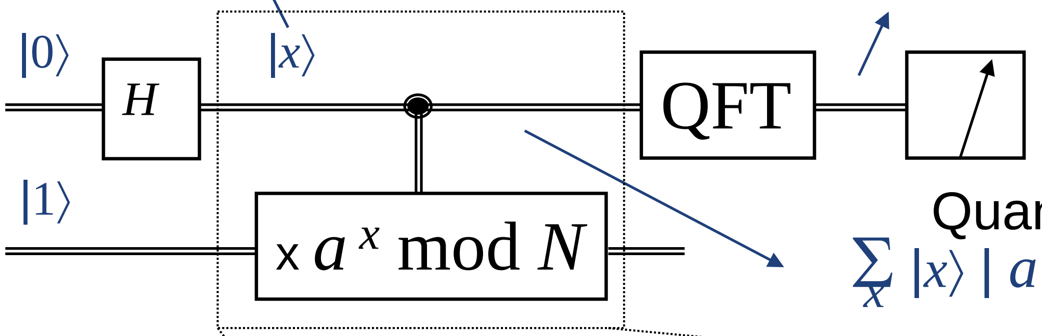
$\sum_k |k2L/r\rangle$ Interference

2 L bits

3 qubits

$L = \log_2(15)$

4 qubits

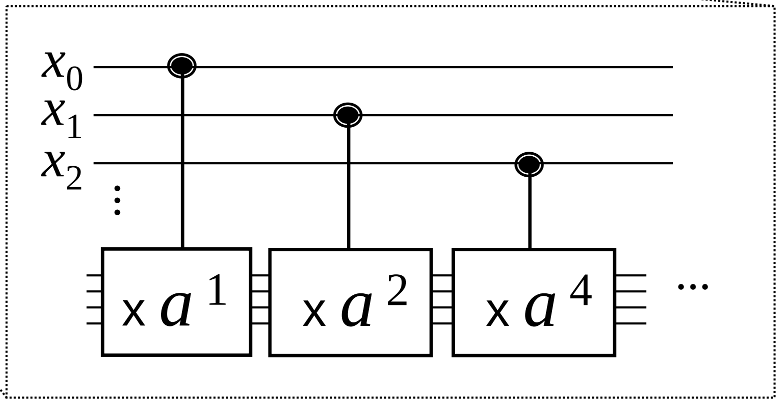


Quantum parallelism

$\sum_x |x\rangle \, | \, a^x \bmod 15 \rangle$

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

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



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

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

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

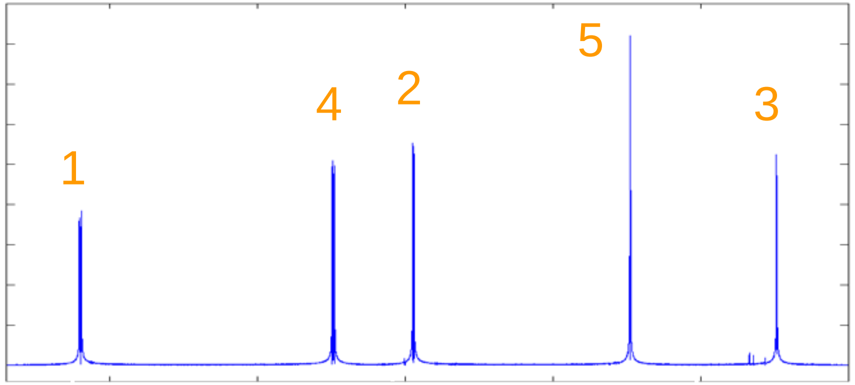
$$|\psi_3\rangle = |0\rangle\,|0\rangle + |1\rangle\,|2\rangle + |2\rangle\,|0\rangle + |3\rangle\,|2\rangle + |4\rangle\,|0\rangle + |5\rangle\,|2\rangle + |6\rangle\,|0\rangle + |7\rangle\,|2\rangle$$

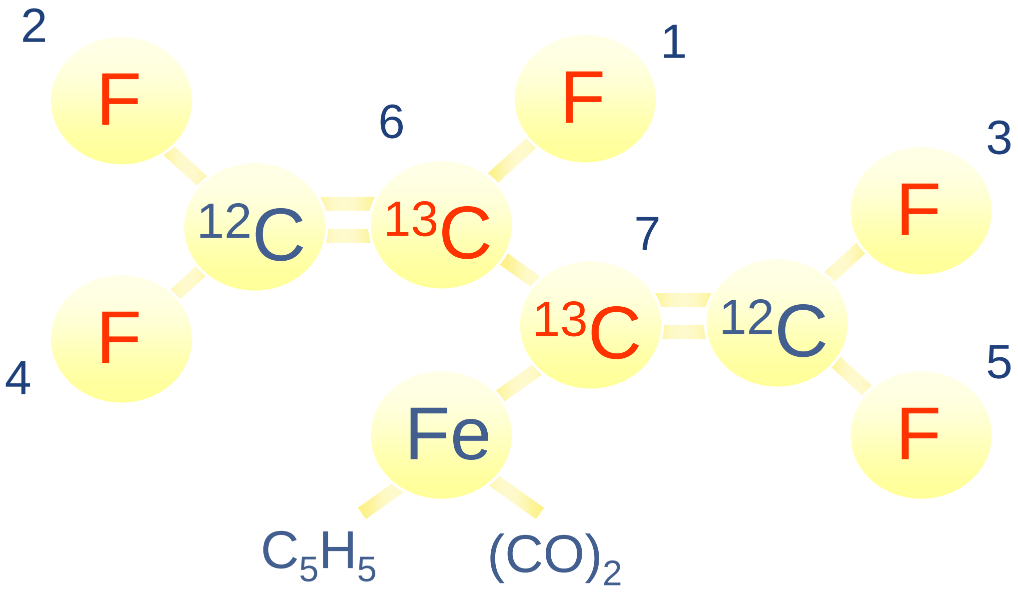
$$= (\,|0\rangle + |2\rangle + |4\rangle + |6\rangle\,)\,|0\rangle + (\,|1\rangle + |3\rangle + |5\rangle + |7\rangle\,)\,|2\rangle$$

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

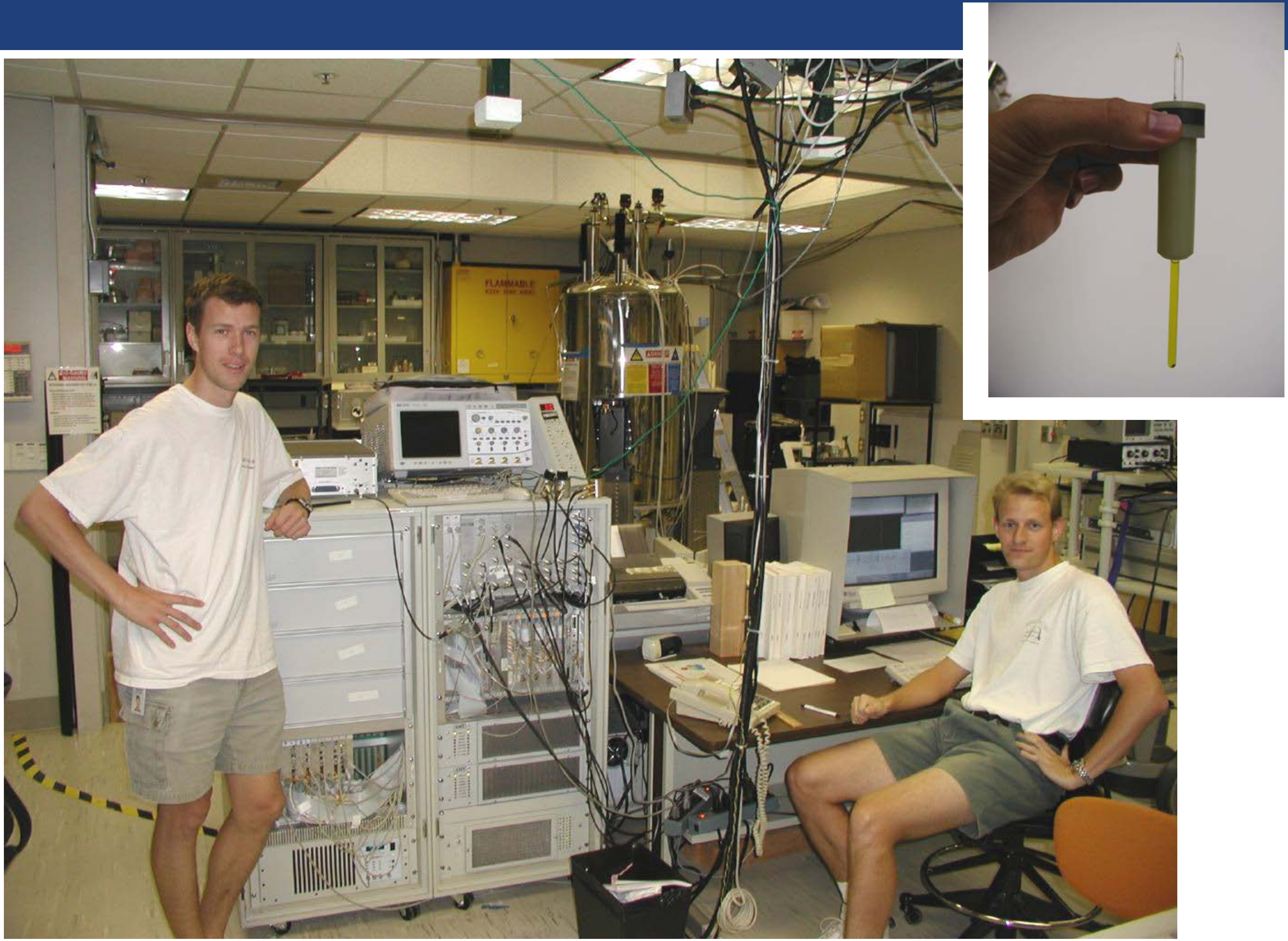
Experimental approach

- 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



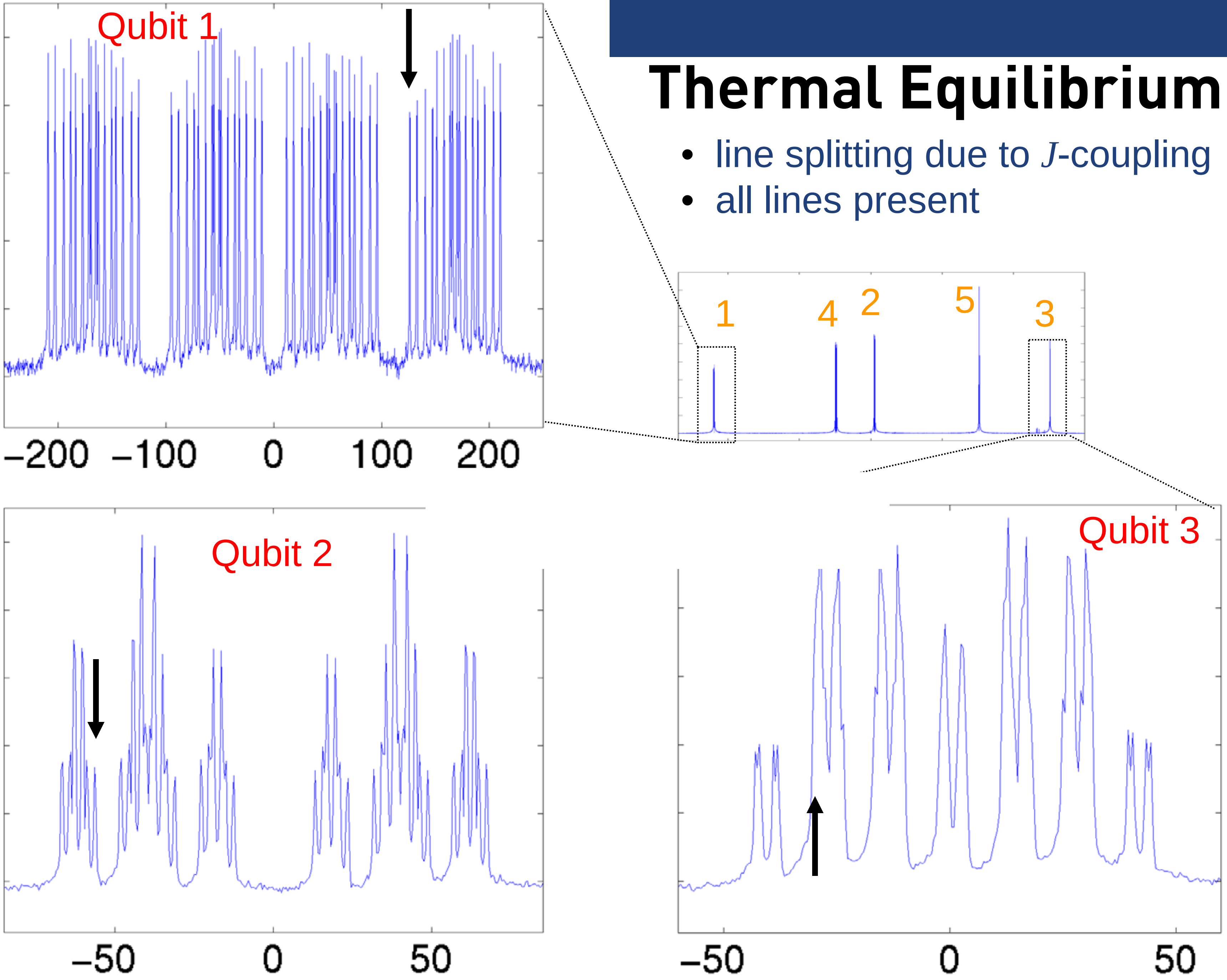


- Larmor frequencies
  - 470 MHz for ^{19}F
  - 125 MHz for ^{13}C
- J - couplings: 2 - 220 Hz
- coherence times: 1.3 - 2 s

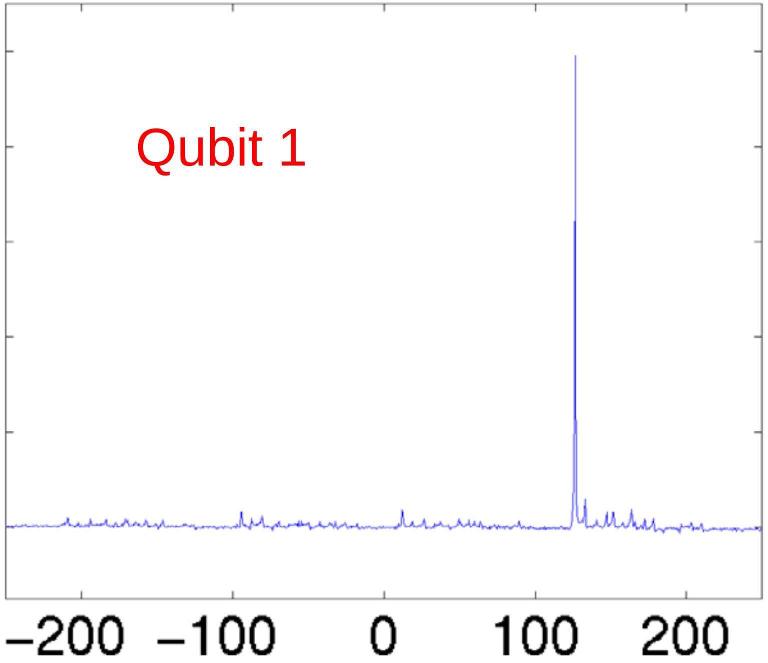

FLAMMABLE

Thermal Equilibrium Spectra

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

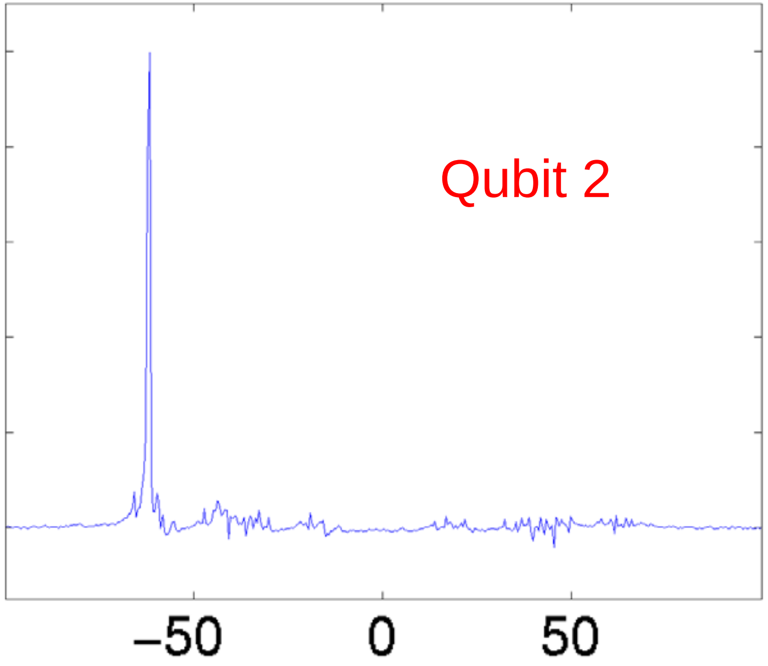


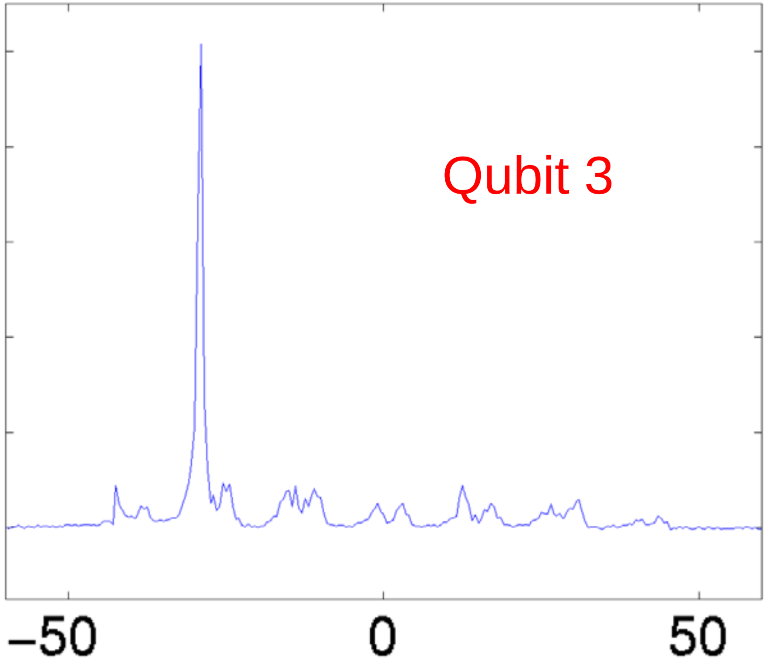
Spectra after state initialization



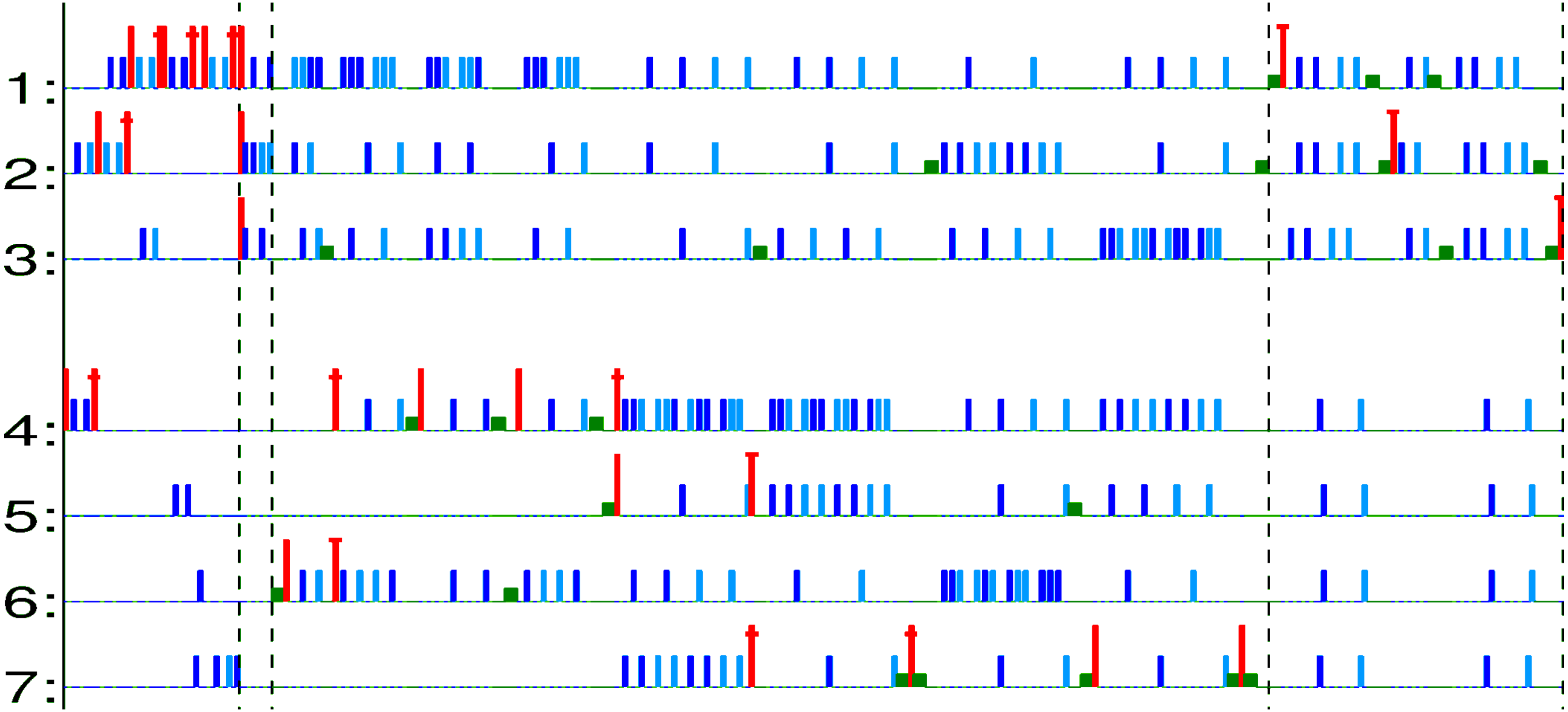
- only the |00 … 0 〉 line remains
- the other lines are averaged away by adding up multiple experiments

RT spins appear cold!





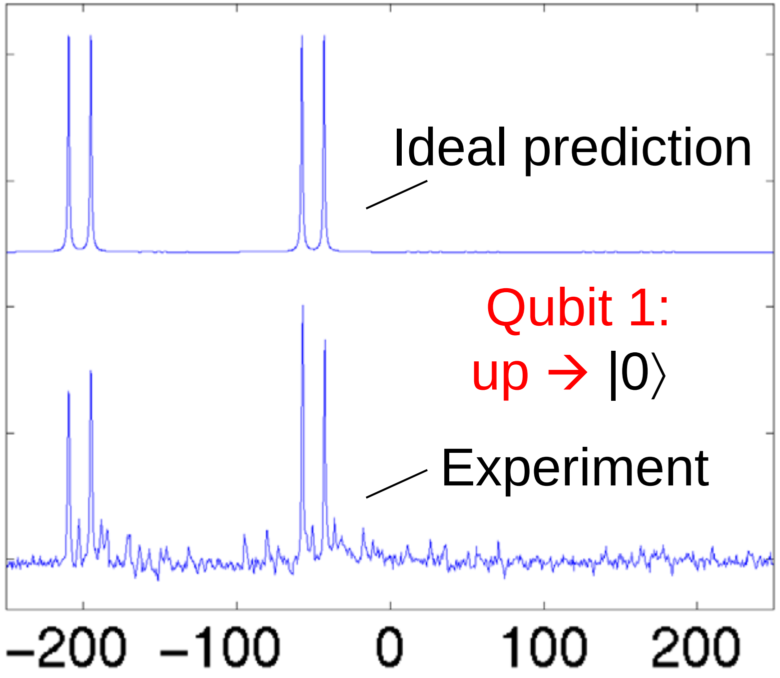
Pulse sequence (a=7)

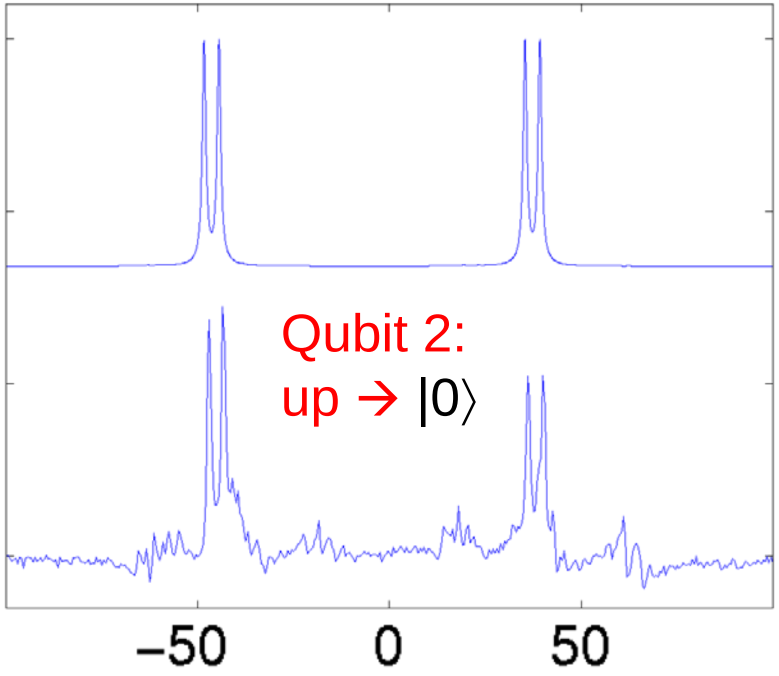


$\pi/2$ X- or Y-rotations (H and gates)
π X-rotations (refocusing)
Z - rotations

> 300 pulses, $\approx$ 720 ms

“Easy” case (a=11)





321	
$\|000\rangle$	0
$\|100\rangle$	4

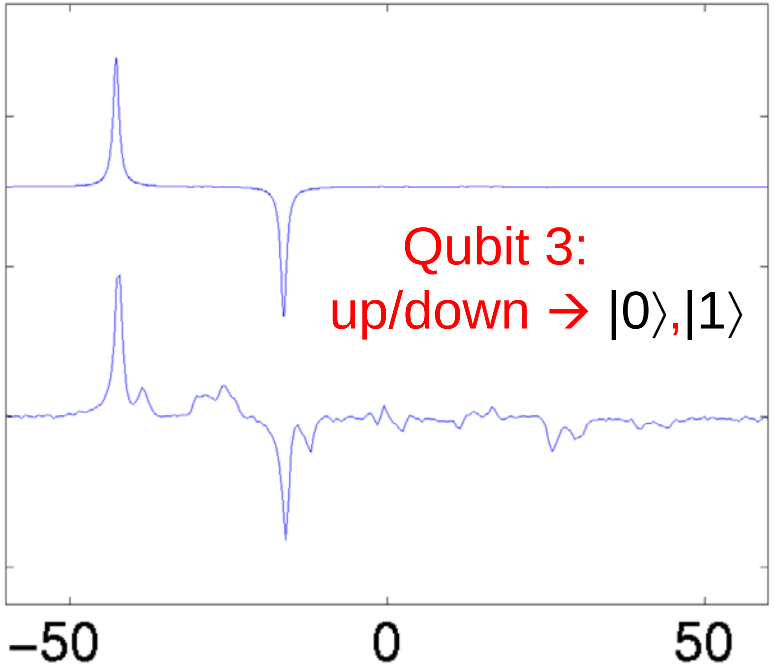
➡ $8 / r = 4$

$r = 2$

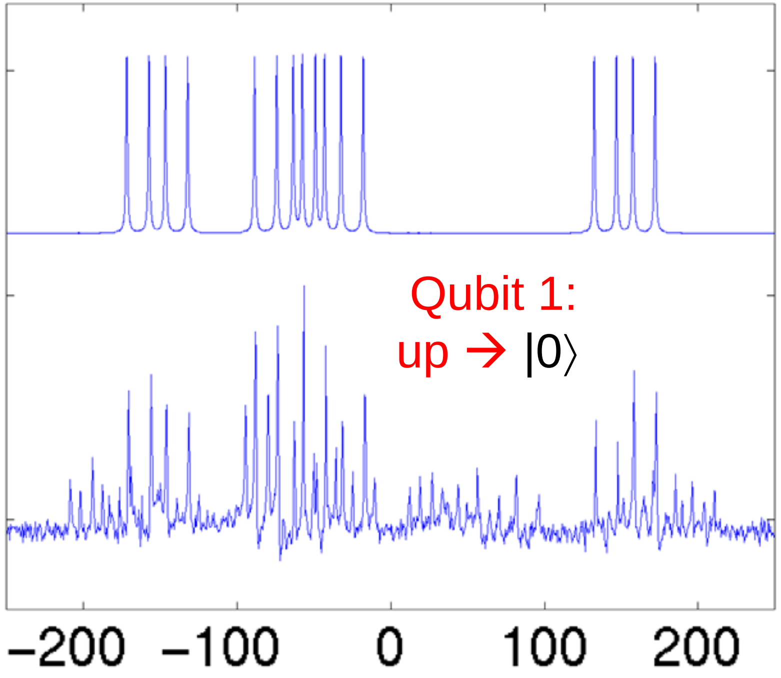
$\gcd(11^{2/2} - 1, 15) = 5$

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

15 = 3 x 5



“Hard” case (a=7)



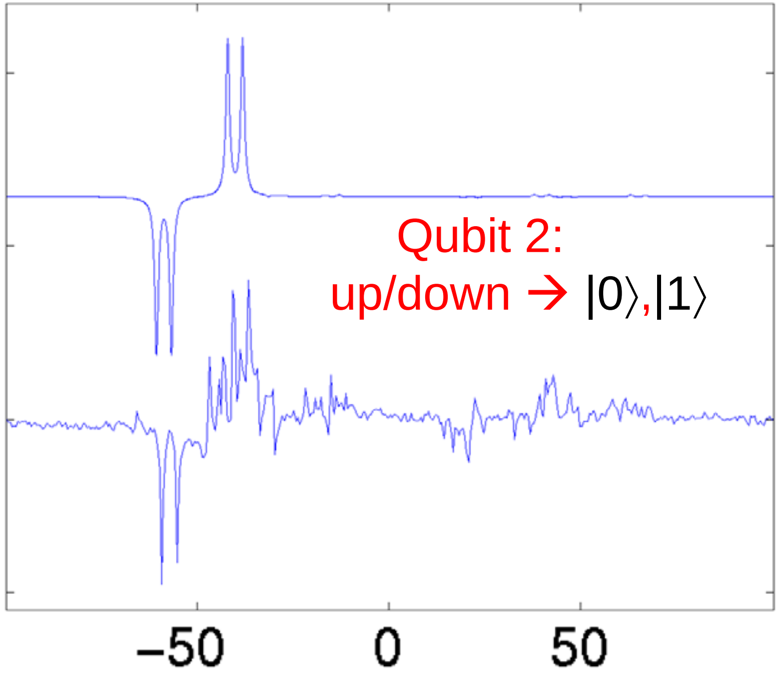
$|000\rangle$ 0
$|010\rangle$ 2
$|100\rangle$ 4
$|110\rangle$ 6

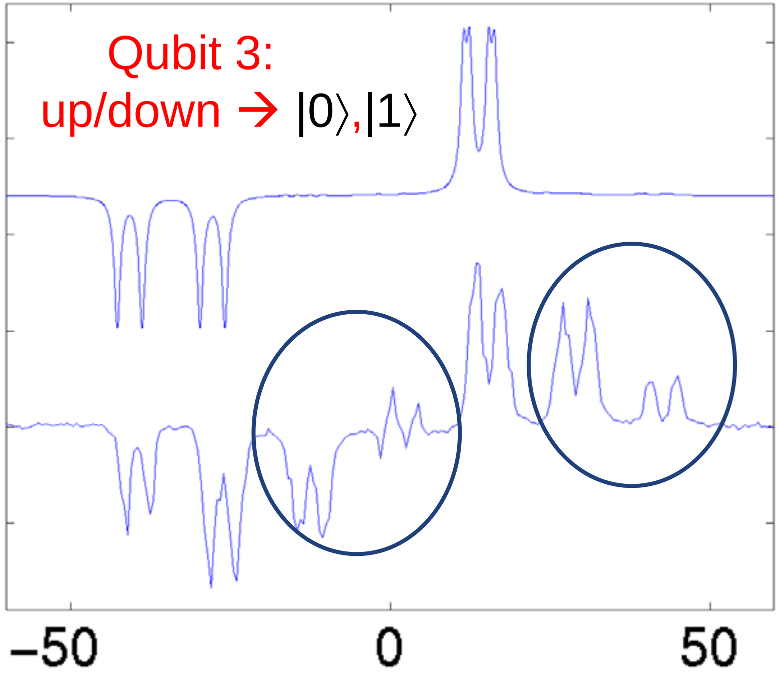
$\Rightarrow$ $8 / r = 2$
$r = 4$

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

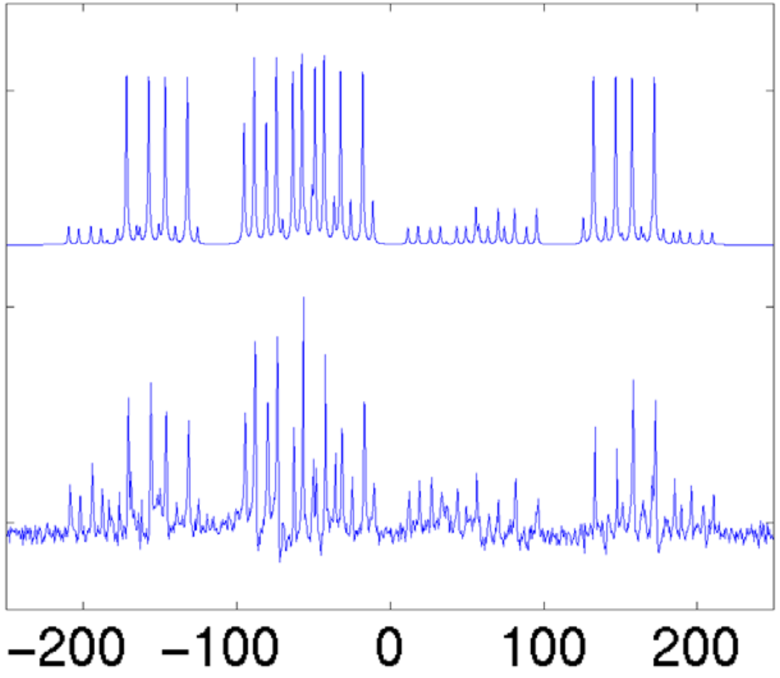
$\gcd(7^{4/2} + 1, 15) = 5$

$15 \cong 3 \times 5$



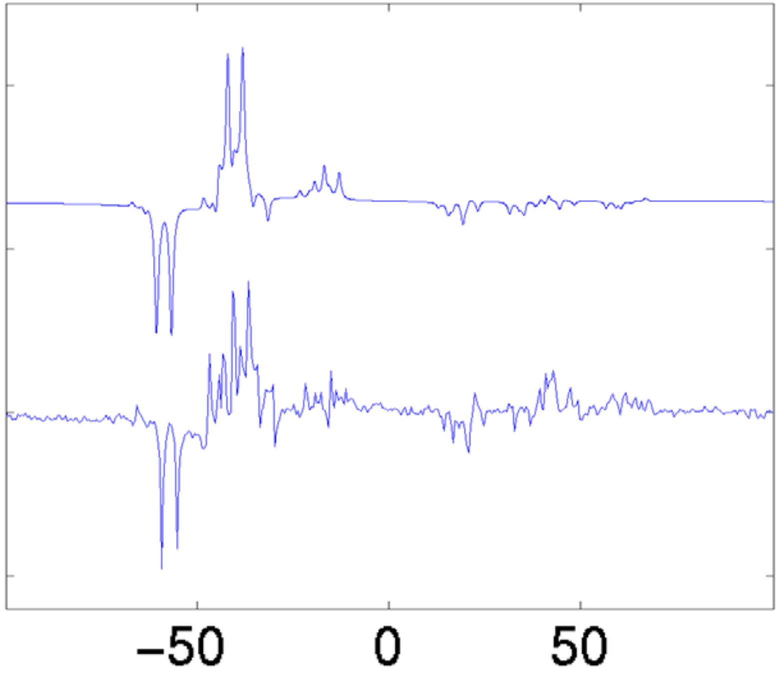


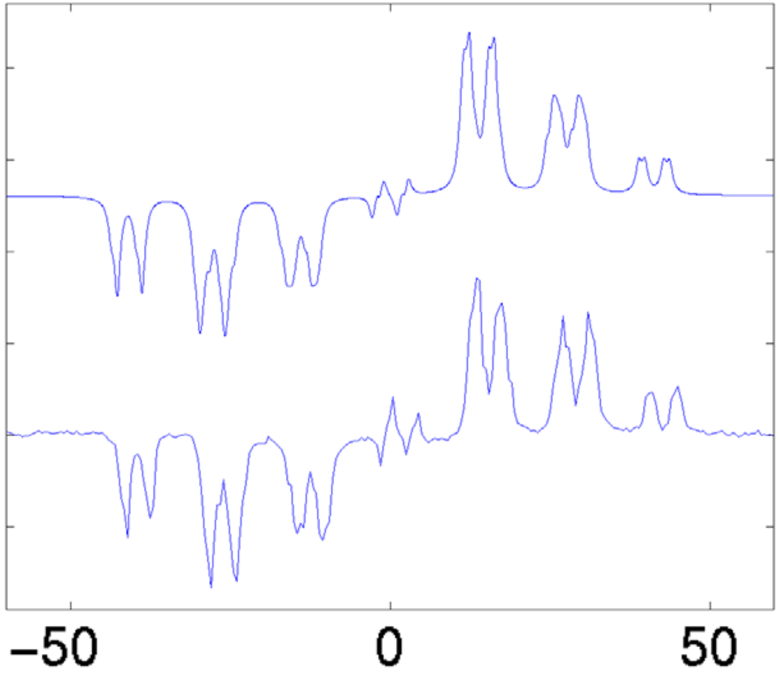
Simulation of decoherence (1)

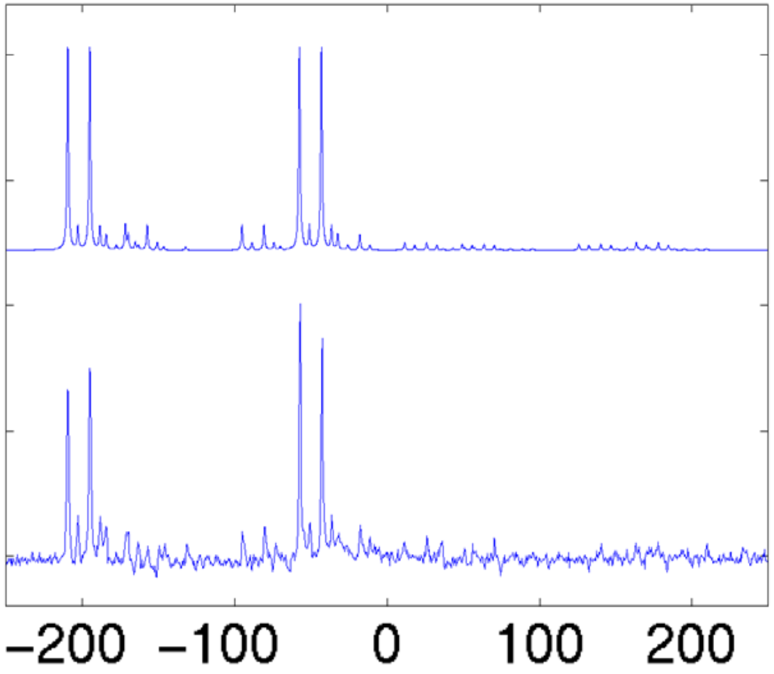


fundamental limit

hard case







Simulation of decoherence (2)

fundamental limit

easy case