Magnetic Resonance in Quantum Information

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Content

Features of (nuclear) magnetic resonance

Brief History of NMR

Example 1:
Liquid-state NMR (=> Factoring of 15)

Example 2:
Quantum information using single spins in diamond

Magnetic nuclei

Blue => Nuclei with spin I = ½
Red => Nuclei with spin I > ½
Grey => Nuclei with spin zero, or not known

Time and Energy scales in NMR & EPR

	Nuclei (Protons)	**Electrons**
• Relevant energy: Zeeman energy in magnetic field (up to ~24Tesla)	43 MHz/T (~0.2μeV/T)	28 GHz/T (~120μeV/T)
• Polarization (room temperature)	~10^{-5}	~1%
• Spin relaxation time T_1	0.1…10^5 s	10^{-9}…1 s
• Spin coherence time T_2	~1…100μs (solids) ~10ms…10s (liquids)	10^{-9}…10^{-3} s
• Spin rotations (pulses)	~1-10μs	~1-100 ns
• Swaps (spin-spin couplings)	~10μs…10ms	~0.1-10μs

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: Boltzmann distribution (room temperature)

✓ Readout: detect spin states with RF coil

✓ Coherence times: easily several seconds
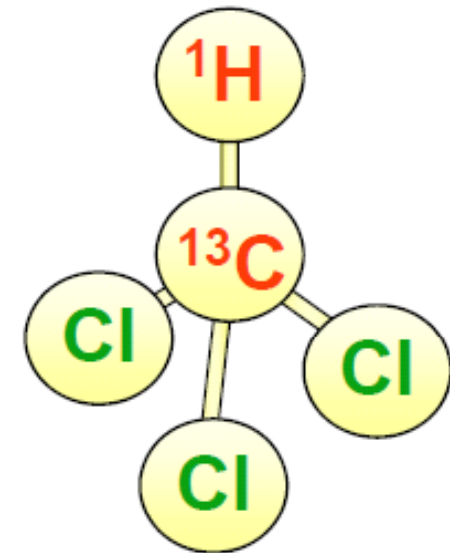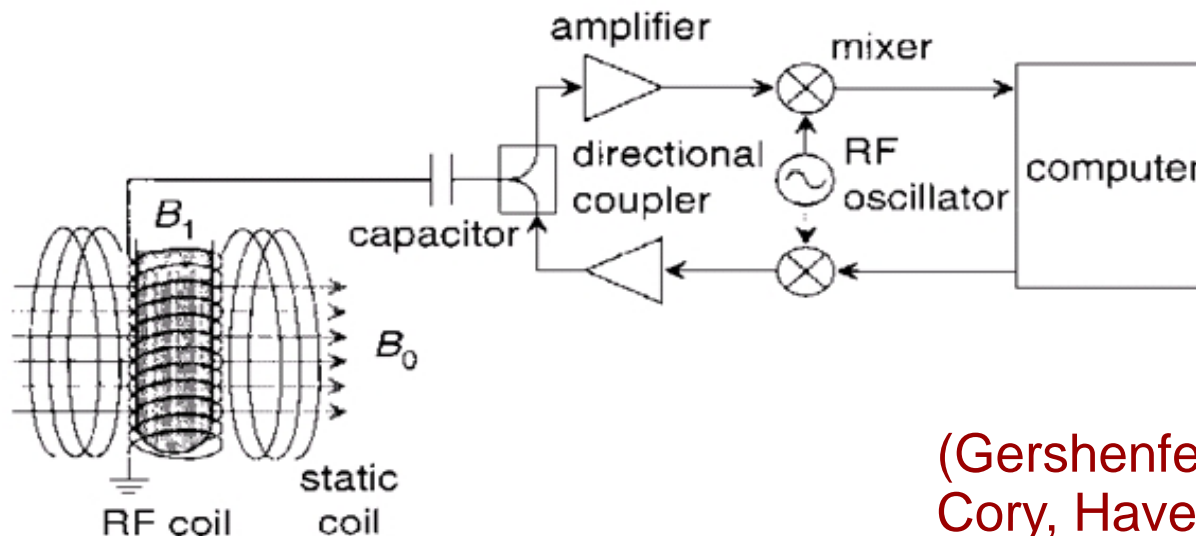
(Gershenfeld & Chuang 1997,
Cory, Havel & Fahmi 1997)

Brief history of NMR

Literature suggestion:
A. Abragam,
"Time reversal: An autobiography"
(Oxford University Press, 1989)

- 1922   Stern-Gerlach experiment
- 1939   Rabi's molecular beam experiment [Nobel Prize 1944]
- 1945-1950   Bloch equations [Nobel Prize 1952]
- 1950-1965   Physical basis of NMR: Relaxation, Couplings, DNP, etc.
- ~1965   Fourier-transform NMR (Ernst) [Nobel Prize 1991]
- 1973   Invention of magnetic resonance imaging [Nobel Prize 2003]
- ~1975   Multi-dimensional NMR
- 1975-1990   Advanced multi-pulse techniques (decoupling, …)
- 1980-   Application in Structural Biology [Nobel Prize 2002]
- 1995 -   Application in Quantum engineering

Example 1: Liquid-state NMR

Principles of NMR QC

Techniques for qubit control

State of the art & Outlook
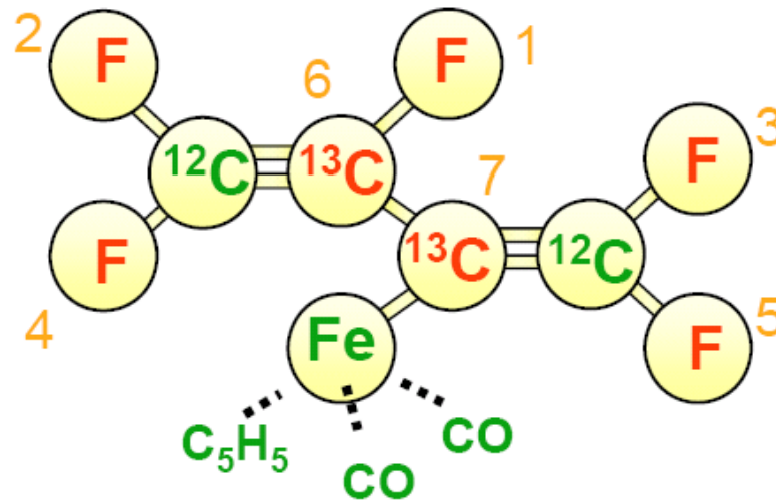
=> "NMR Quantum Computing"

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

How to factor 15 with NMR?

perfluorobutadienyl
iron complex

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

Liquid-state NMR

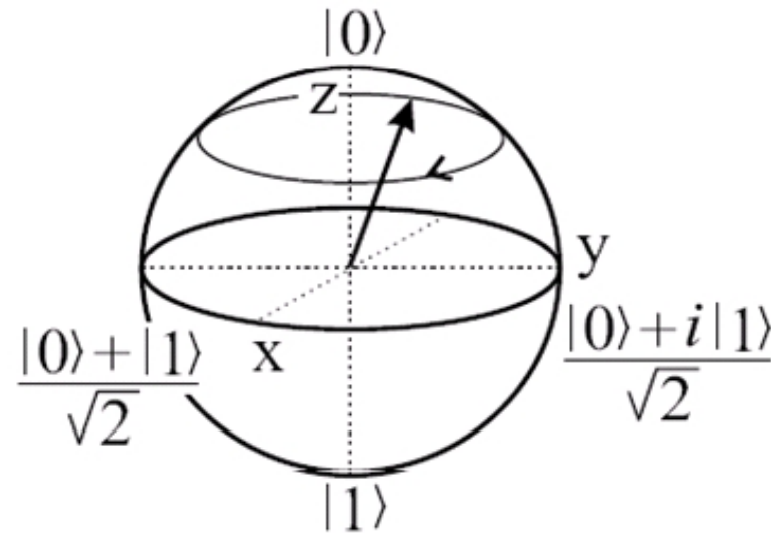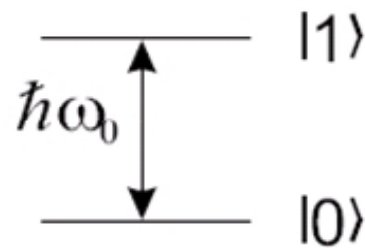Survey of NMR quantum computing

⟹ Principles of NMR QC

Techniques for qubit control

Summary: Pros & Cons

Nuclear spin Hamiltonian
Single spin ½

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

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

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

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

gyromagnetic (g-)factor: γ

Nuclear spin Hamiltonian
Multiple spins

without qubit/qubit coupling

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

F_3 F_1 F_5
C—C C
F_2 C—C F_4
Fe
$(CH)_5$ $(CO)_2$

chemical shifts
of the five F qubits
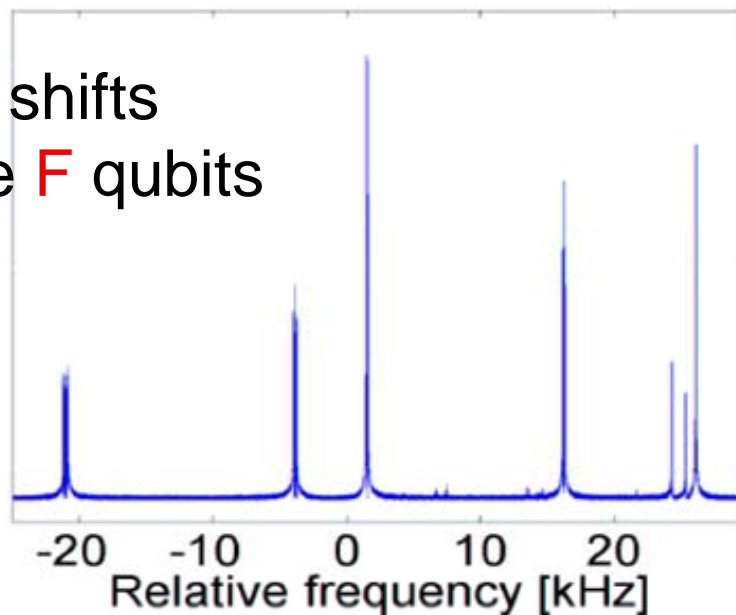
	MHz	
$_1H$	500	~ 25 mK
$_{13}C$	126	
$_{15}N$	-51	
$_{19}F$	470	
$_{31}P$	202	

(at 11.7 Tesla)
qubit level separation

Hamiltonian with RF field
single-qubit rotations

σz   σx   σy

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

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

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

rotating wave approximation   typical strength I_x, I_y : up to 100 kHz
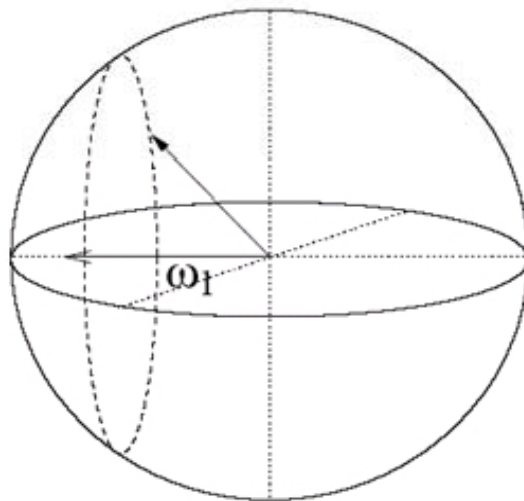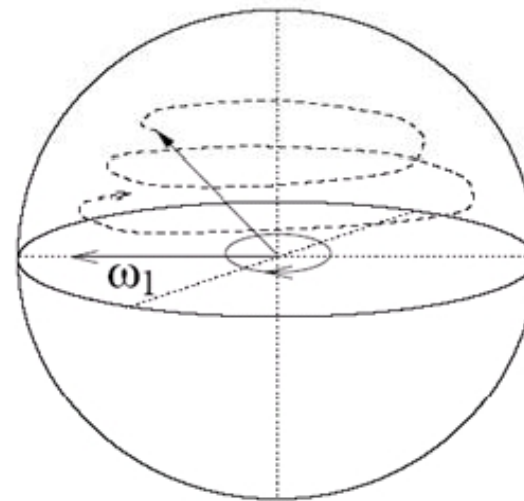
Rotating frame   Lab frame

Nuclear spin Hamiltonian
Coupled spins

J>0: antiferro mag.

J<0: ferro-mag.

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

F_3 F_1 F_5 C—C F_2 C—C F_4 Fe $(CH)_5$ $(CO)_2$

16 configurations

$|1\rangle|1\rangle$

ω_0^2

$\omega_0^1 + \pi J$

$|1\rangle|0\rangle$

$|0\rangle|1\rangle$

ω_0^1

$\omega_0^2 - \pi J$

$\pi J/2$

$|0\rangle|0\rangle$
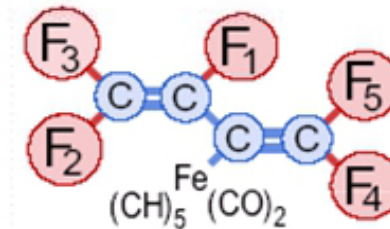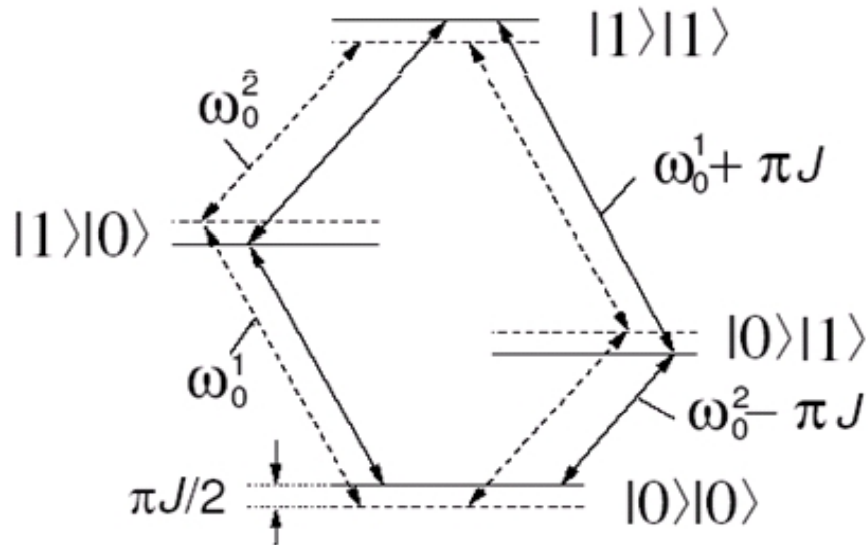
solid (dashed) lines are (un)coupled levels

Amplitude real part [a.u.]

1000 1010 1001 1011 1100 1110 1101 1111

0000 0010 0001 0011 0100 0110 0101 0111

-50   0   50
Relative frequency [Hz]

8
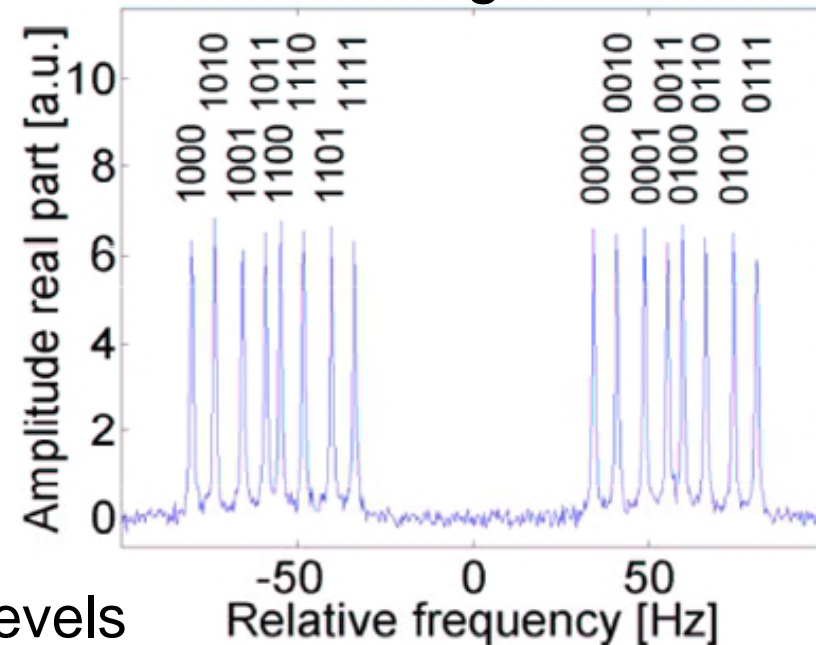
Controlled-NOT in NMR

γ_{12} δ_{12}

ν

ν_1 ν_2

$|\uparrow\rangle_2$ $|\downarrow\rangle_2$

A target bit
B control bit

$|0\rangle$

$\dfrac{|0\rangle + i|1\rangle}{\sqrt{2}}$

$\dfrac{|0\rangle + |1\rangle}{\sqrt{2}}$

$|1\rangle$

Before		After	
A	B	A	B

" flip A if B ↓ "

wait
Delay
$1/2J_{AB}$

Y^A_{90} X^A_{90}
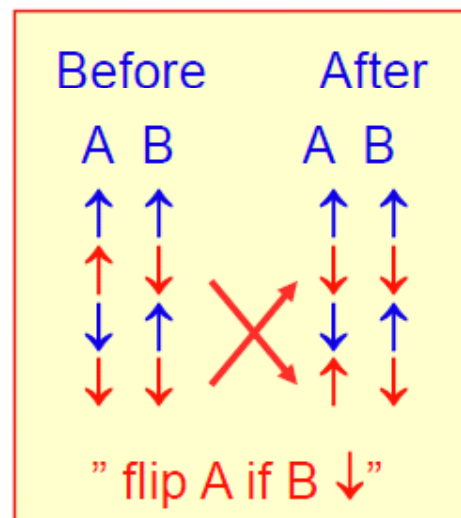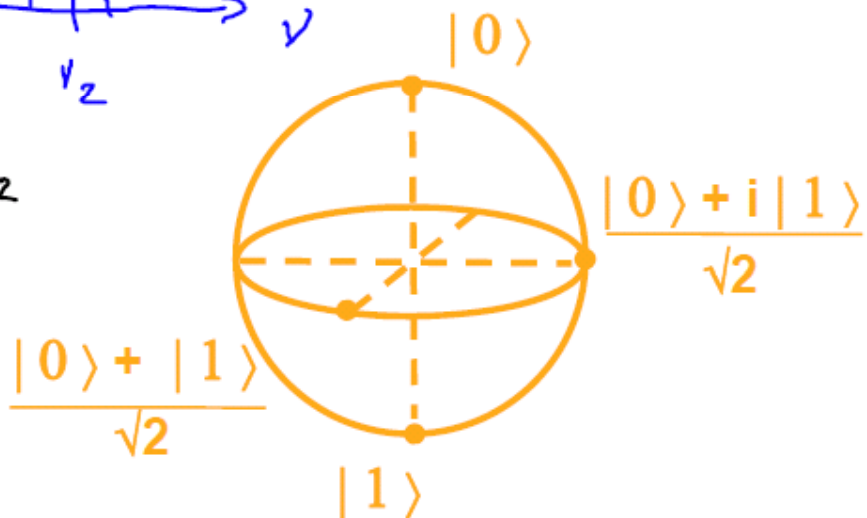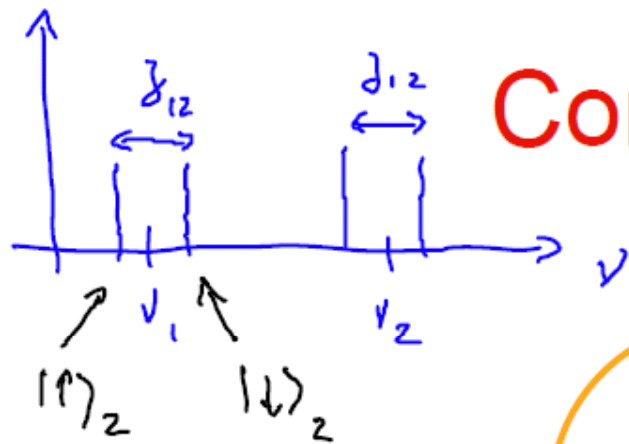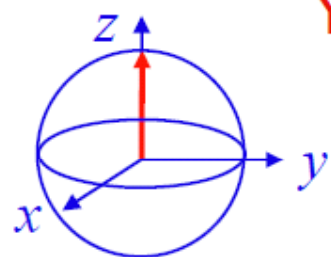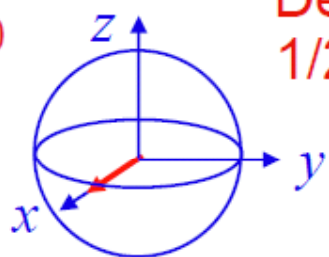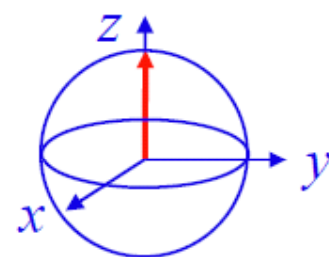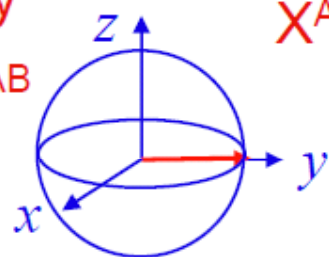
if spin B is ↑

if spin B is ↓
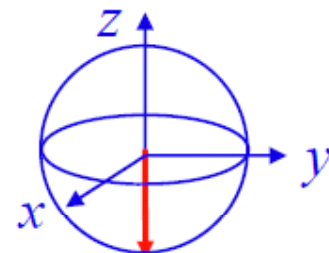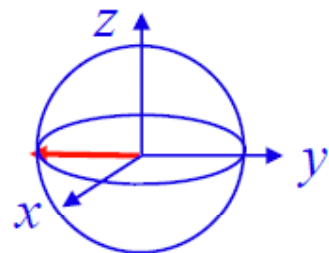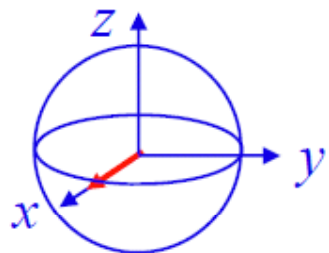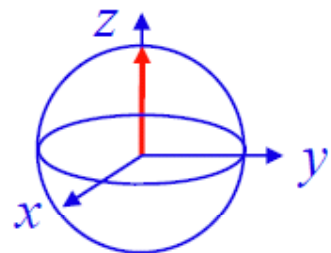
different rotation direction depending on control bit ⟶ time

9

Making room temperature spins look cold

warm ↑↑   ↑↓   ↓↑   ↓↓

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

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

low energy   high energy

↑↑

cold

↑↓   ↓↑   ↓↓

equalize population

↑↑
↑↓   ↓↑   ↓↓

quasi cold

Look exactly like cold spins !

warm

[Hz]
−200 −100   0   100   200

quasi cold

[Hz]
−200 −100   0   100   200
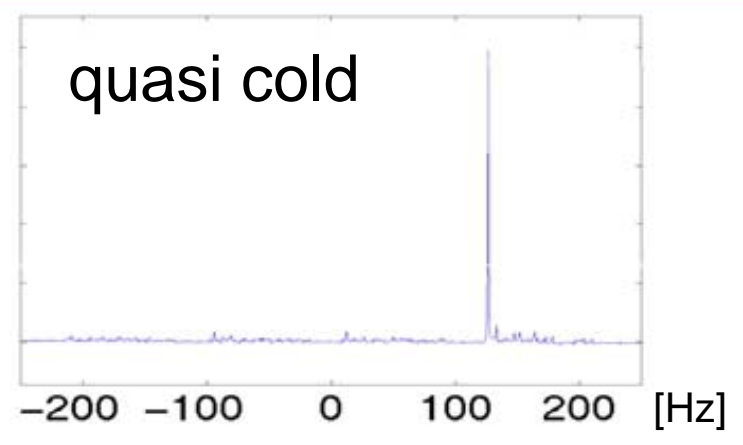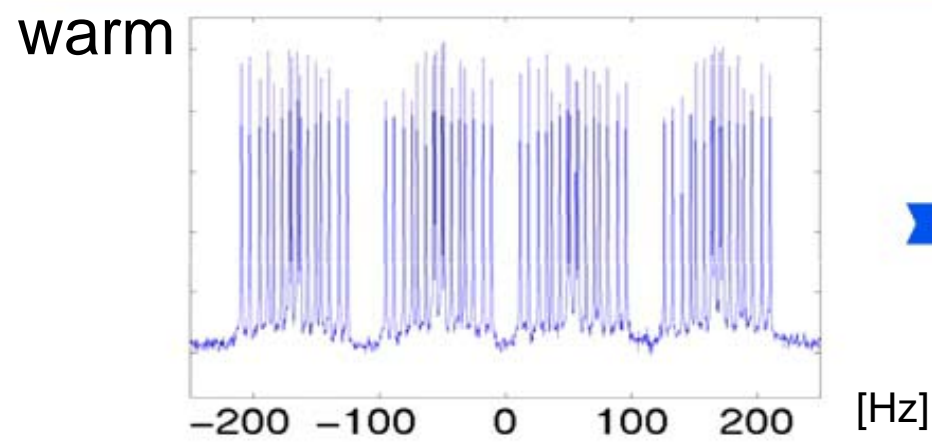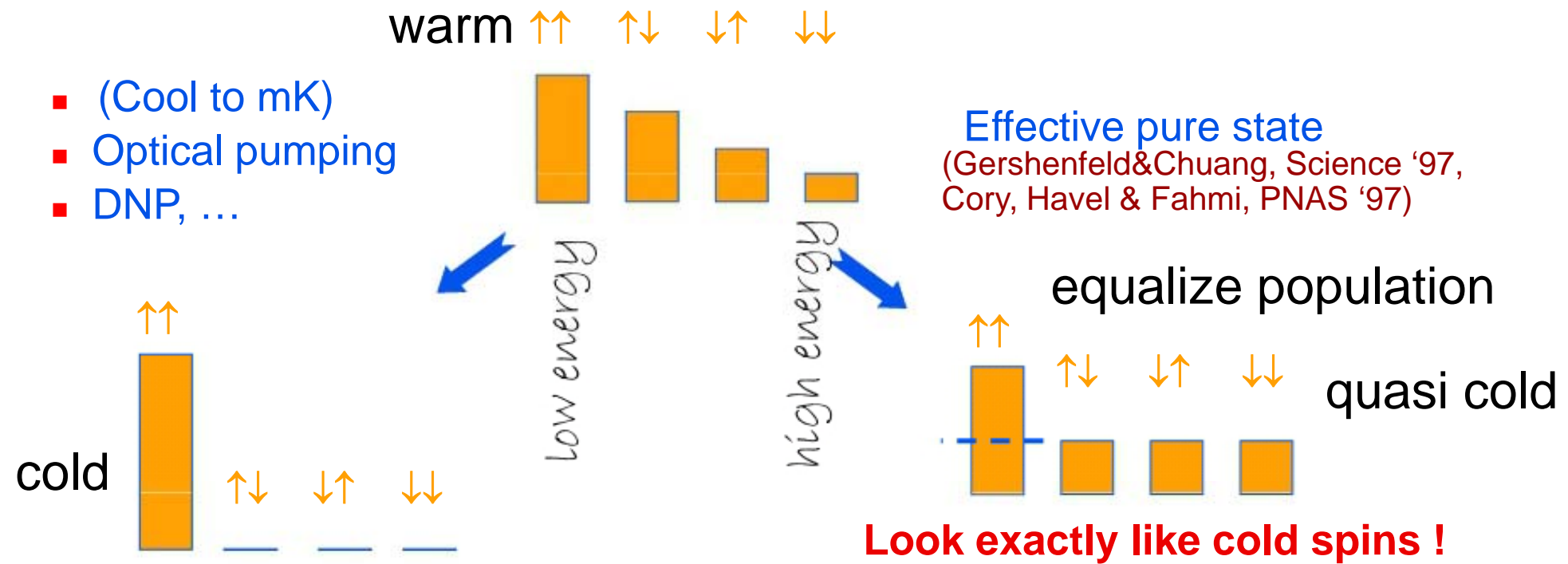
Effective pure state preparation

(1) Add up 2^N-1 experiments (Knill,Chuang,Laflamme, PRA 1998)
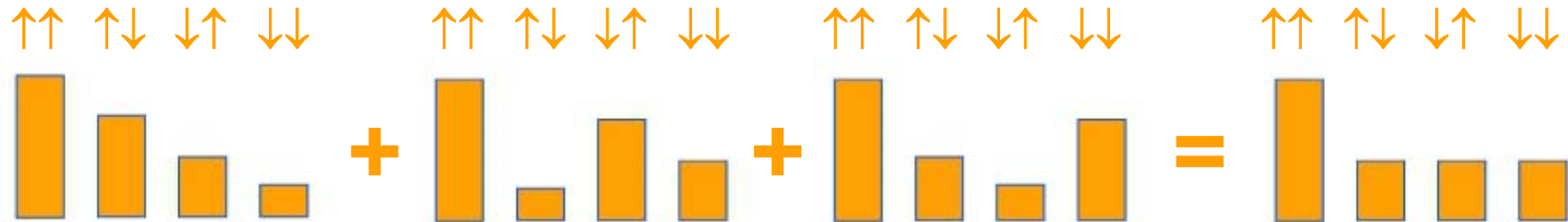
Later : $(2^N - 1) / N$ experiments (Vandersypen *et al.*, PRL 2000)

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
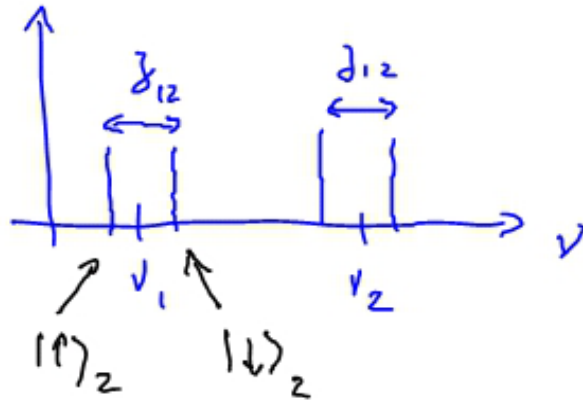
Phase sensitive detection
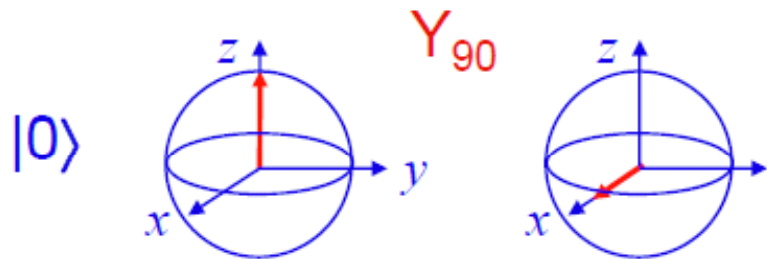
positive signal for |0> (in phase)
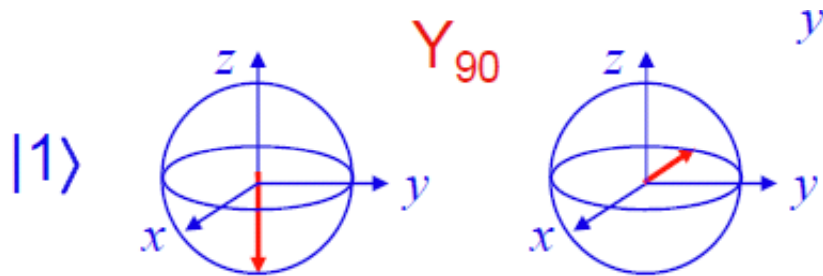
negative signal for |1> (out of phase)
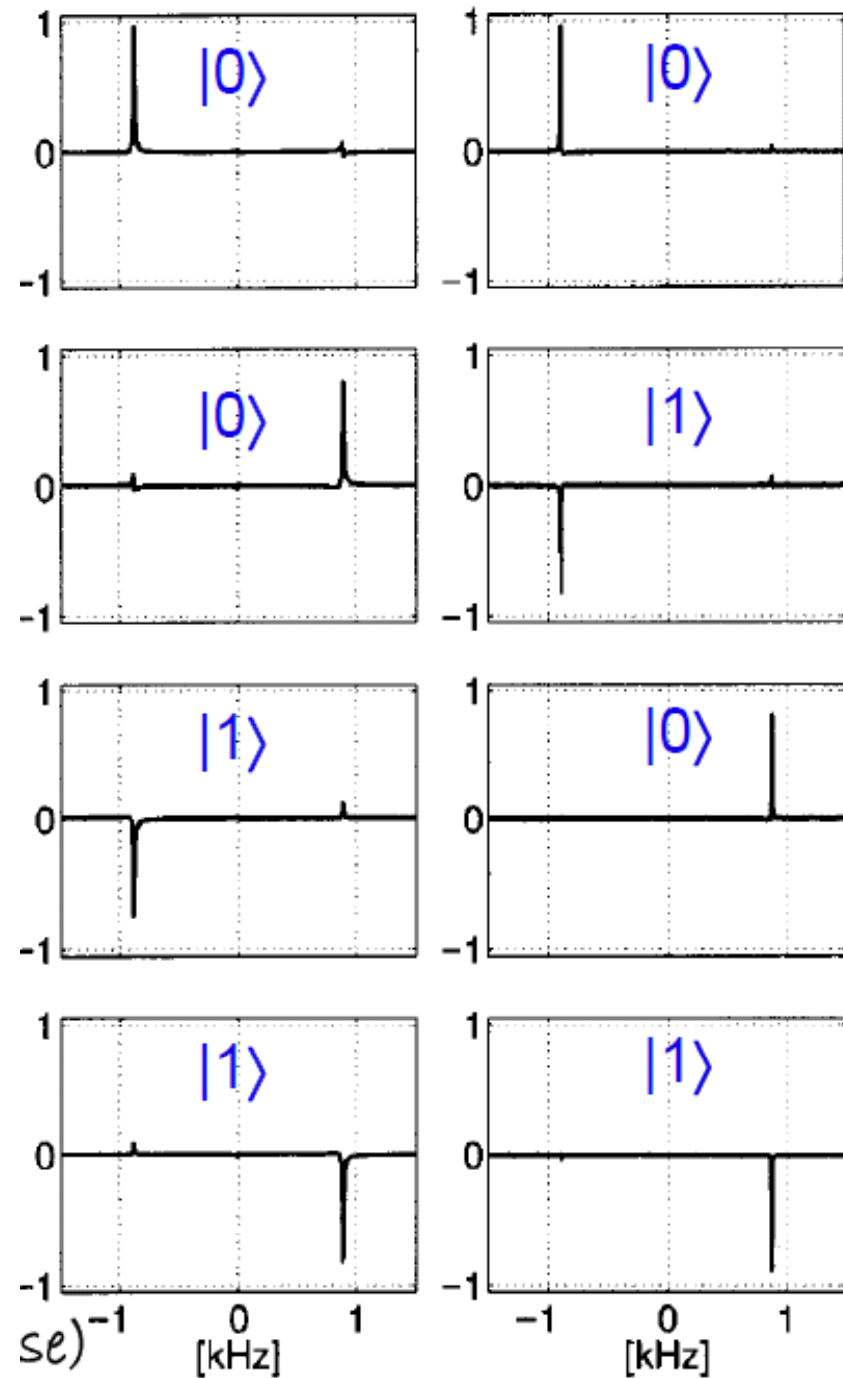
NMR Spectrometer

Computer – Console – Superconducting magnet

Transmission / Receiver coil

Liquid-state NMR

Survey of NMR quantum computing

Off-resonance pulses and spin-selectivity

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

spectral content of a square pulse

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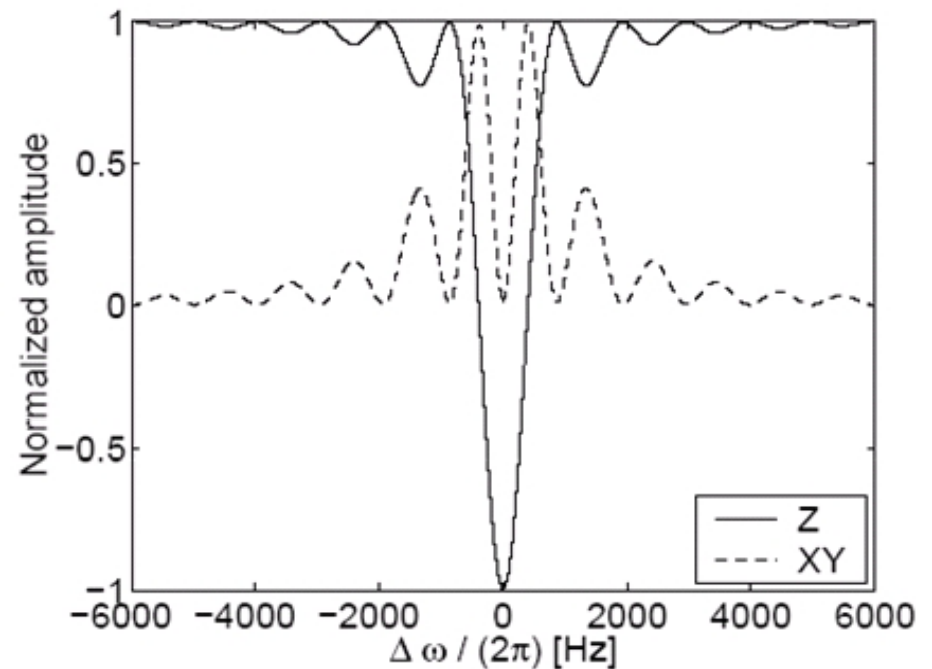
may induce transitions in other
qubits

Pulse shaping for improved spin-selectivity

gaussian pulse profile
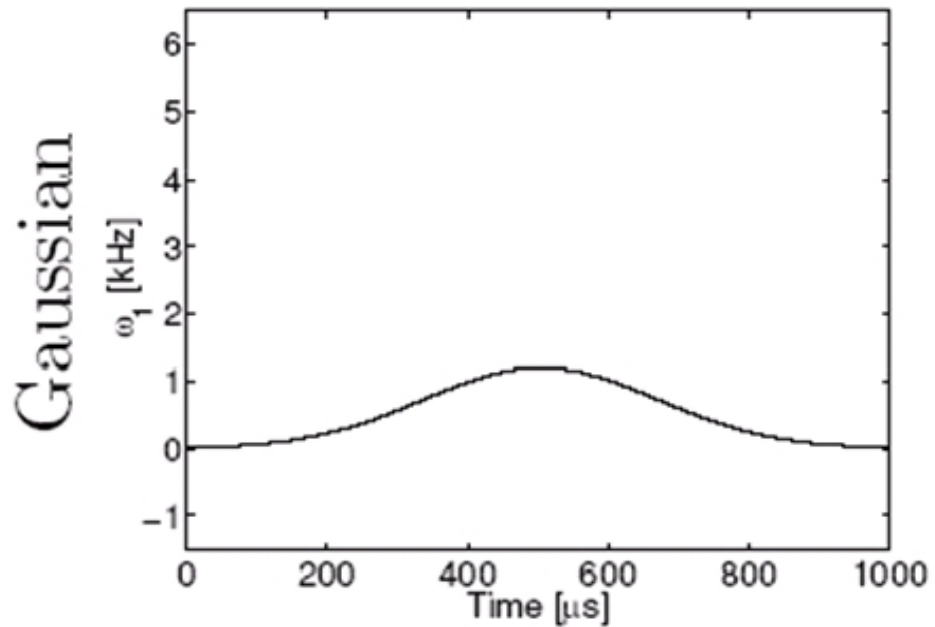
gaussian spectrum
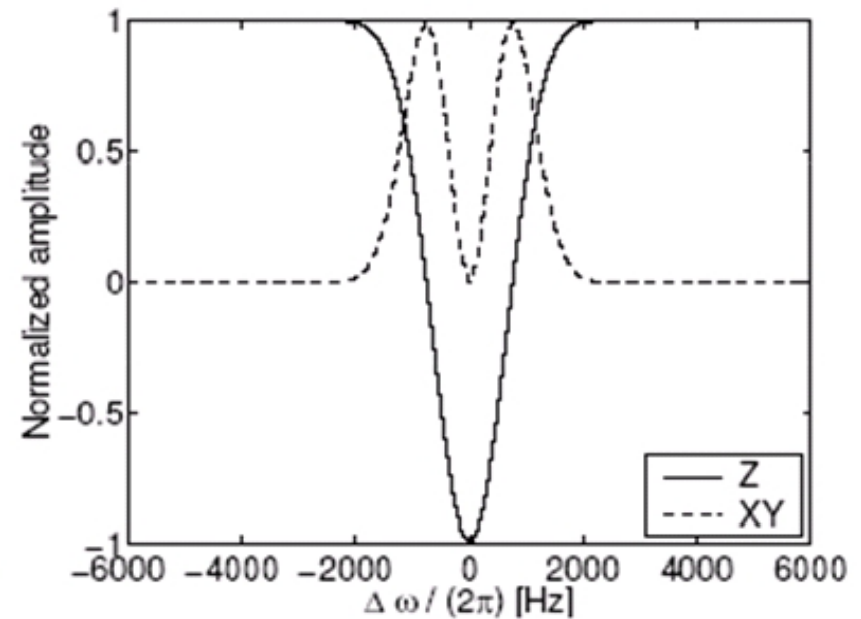
less cross-talk

Missing coupling terms: Swap

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

Missing couplings: swap states along qubit network

$$SWAP_{12} = CNOT_{12}\ CNOT_{21}\ CNOT_{12}$$
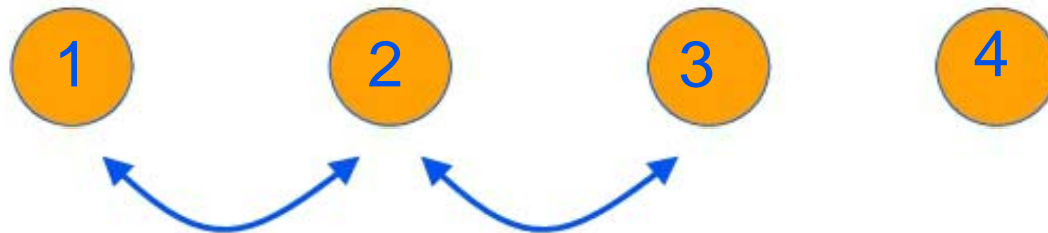
"only" a linear overhead ...

Undesired couplings: refocus
remove effect of coupling *during delay times*

opt. 1: act on qubit B
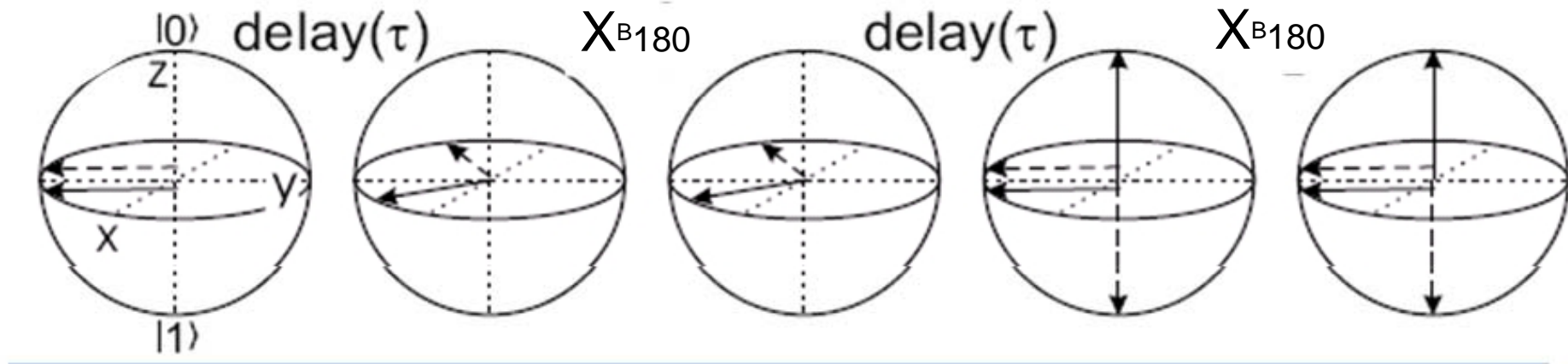
opt. 2: act on qubit A

- 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
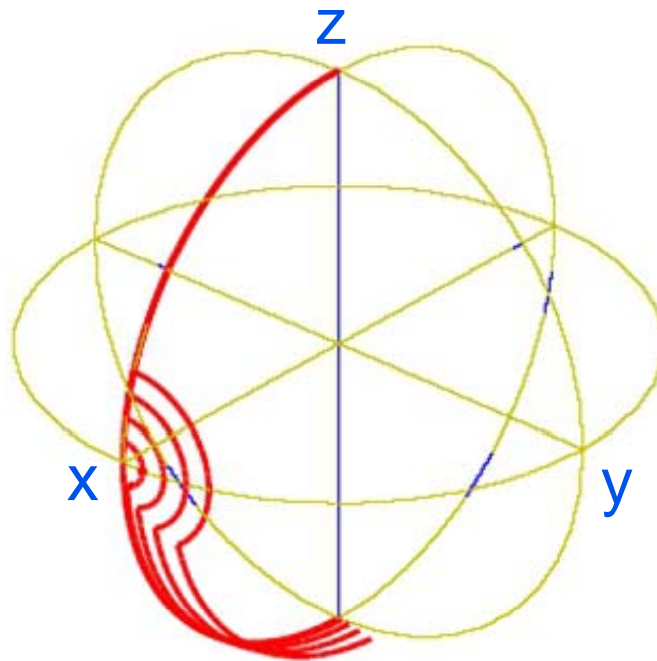
corrects for
off-resonance
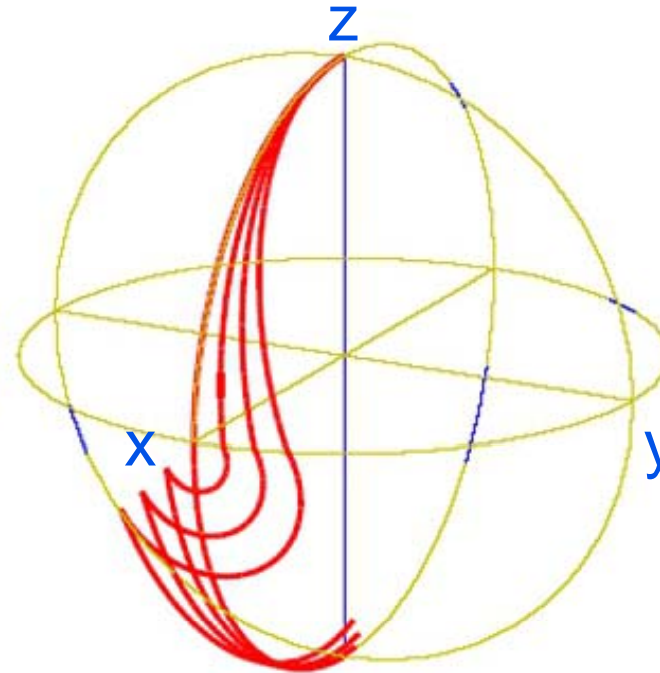
However: doesn't work for arbitrary input state
But: there exist composite pulses that work for all input states

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
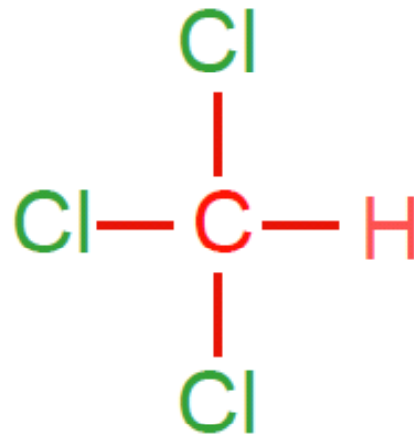
Q. Error correction
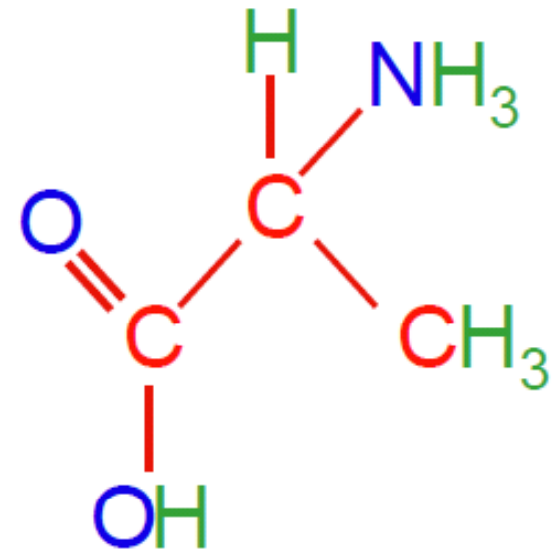
Logical labeling / Grover
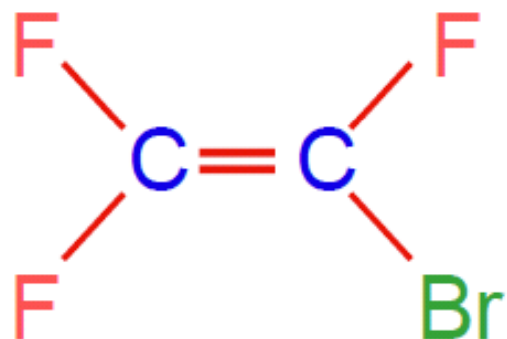
Teleportation
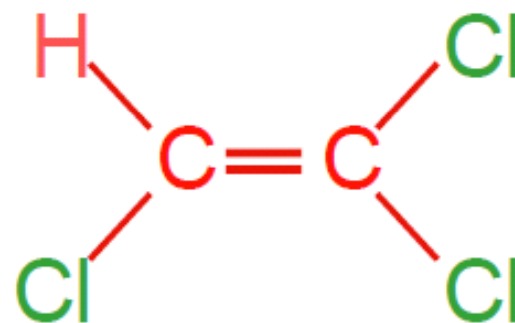
Q. Error Detection
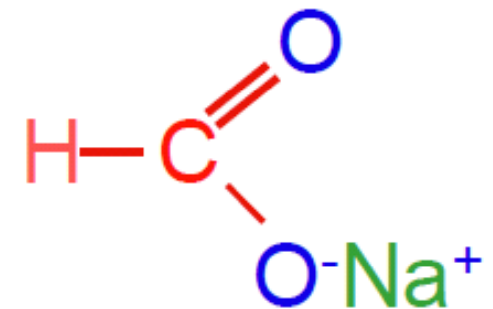
Quantum computer molecules (2)

Deutsch-Jozsa
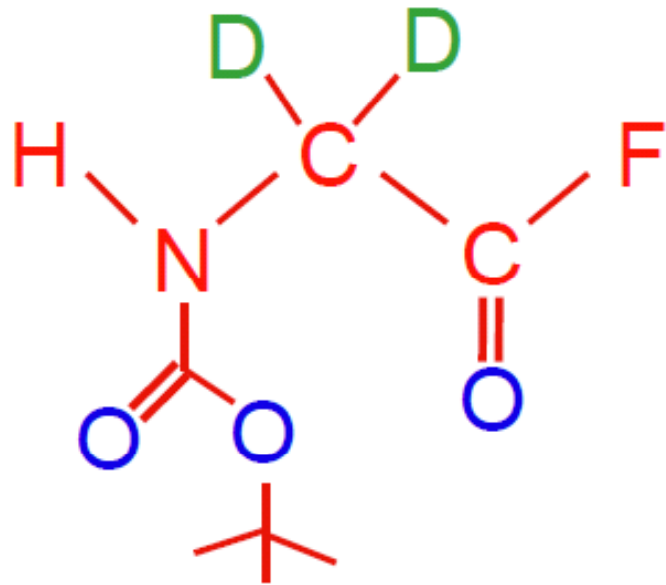
7-spin coherence
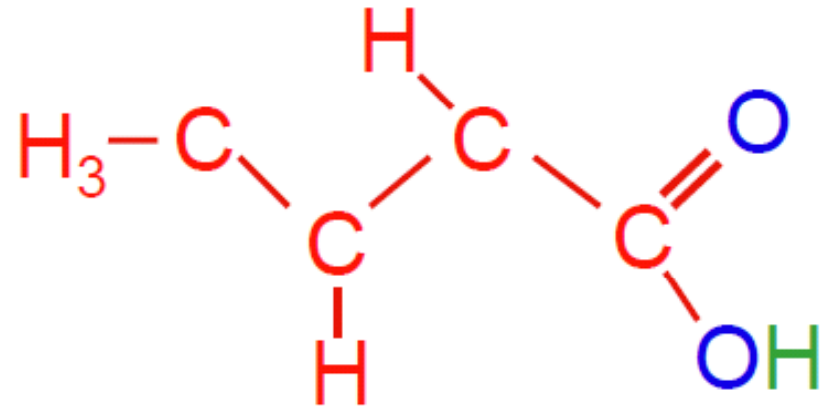
Order-finding
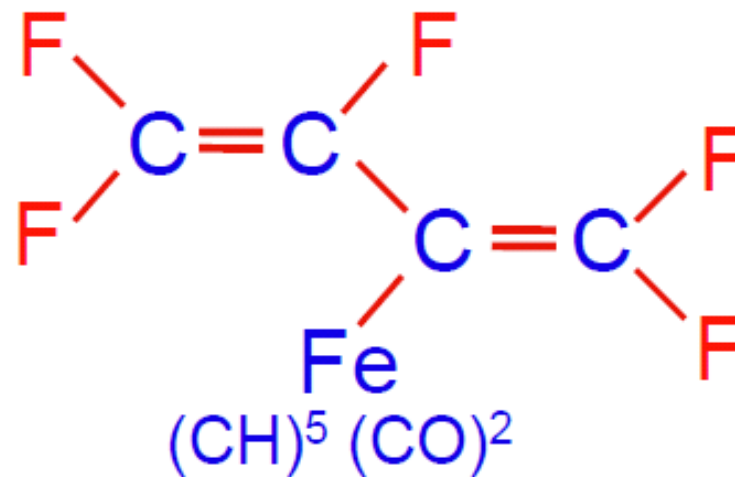
$(CH)^5 (CO)^2$

Liquid-state NMR

Survey of NMR quantum computing

Principles of NMR QC

Techniques for qubit control

➡ Summary: Pros & Cons

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

The main issue: 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 coupling during RF pulses

Finally

decoherence

Electron spin qubits
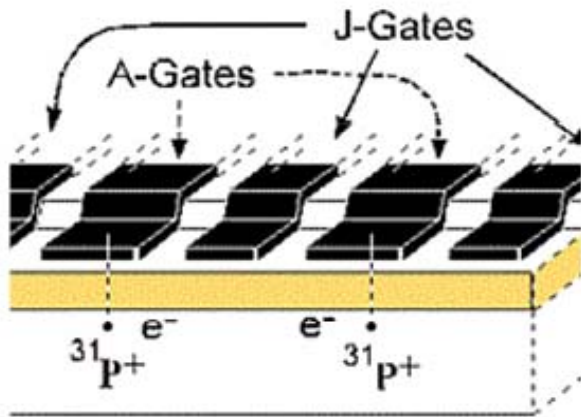
Kane, Nature 1998
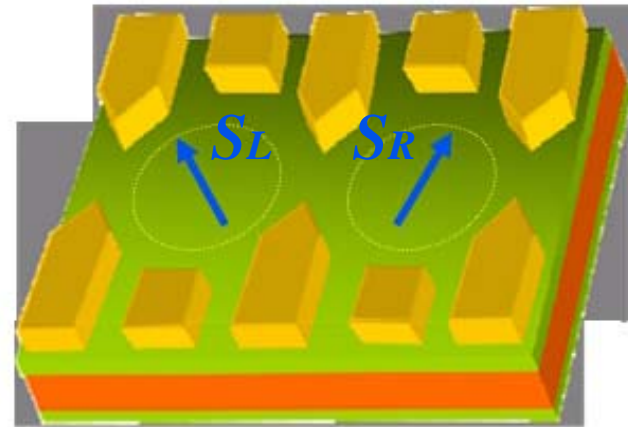
Loss & DiVincenzo, PRA 1998
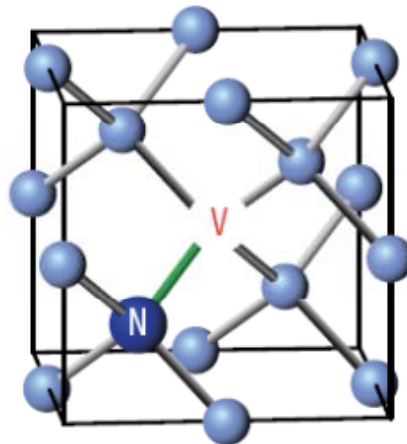
Gruber, Science, 1997

Quantum information using single spins in diamond

Literature hint:

F. Jelezko, J. Wrachtrup,
"Single defect centres in diamond: A review"
Phys. stat. sol. (a) 203, 3207 (2006).

Single spins in diamond

Diamond nitrogen vacancy center (NV Center)
- Principles of Optically-detected magnetic resonance (ODMR)
- Initialization, manipulation, read-out of NV electron spin

Environment: Diamond host material

Applications

Optically-detected magnetic resonance (ODMR)

Idea: Detect optical instead of microwave/radio-frequency photons

Requirement: Optical photon must be correlated with spin state

$\sigma = \uparrow$ or $\downarrow$

Intensity I
Wavelength λ
Polarization P

Intensity $I'(\sigma)$
Wavelength $\lambda'(\sigma)$
Polarization $P'(\sigma)$
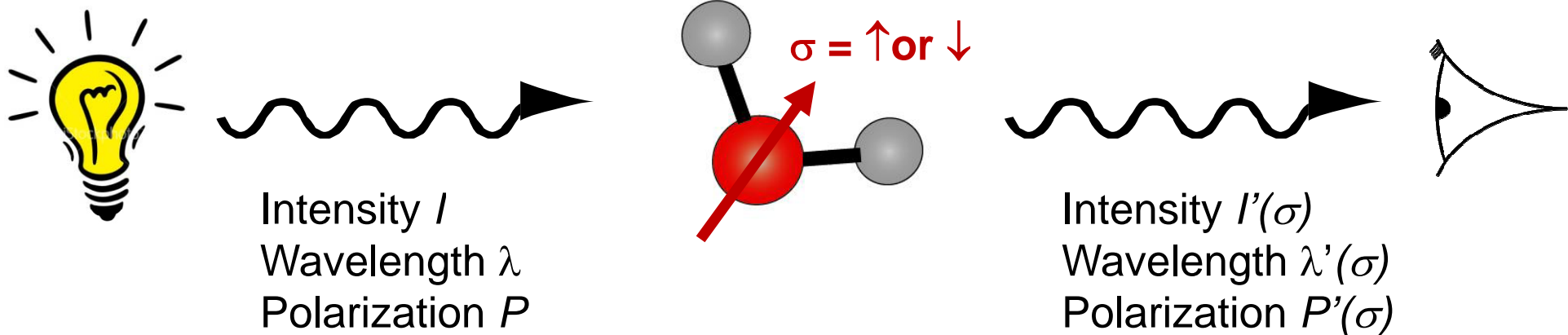
Optically detected magnetic resonance

Some History

- Optical detection of paramagnetism in phenantren (Kwiram, 1967)

  (… 1980ies: Invention of single molecule spectroscopy …)

- Optical detection of magnetic resonance in a single pentacene molecule
  Wrachrup, Moerner (1993)
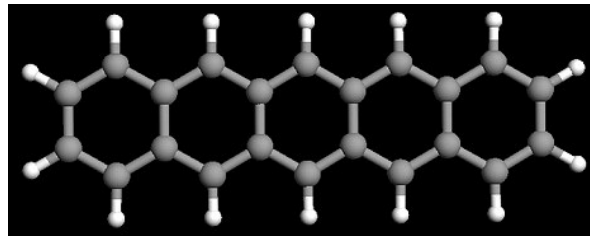
- Optical detection of single nitrogen vacancy centers in diamond:
  Gruber, Wrachtrup (1997)
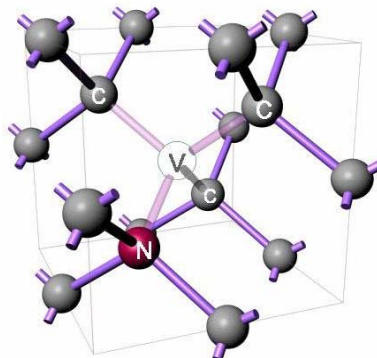
Single spin detection of NV centers

Gruber, Science 1997
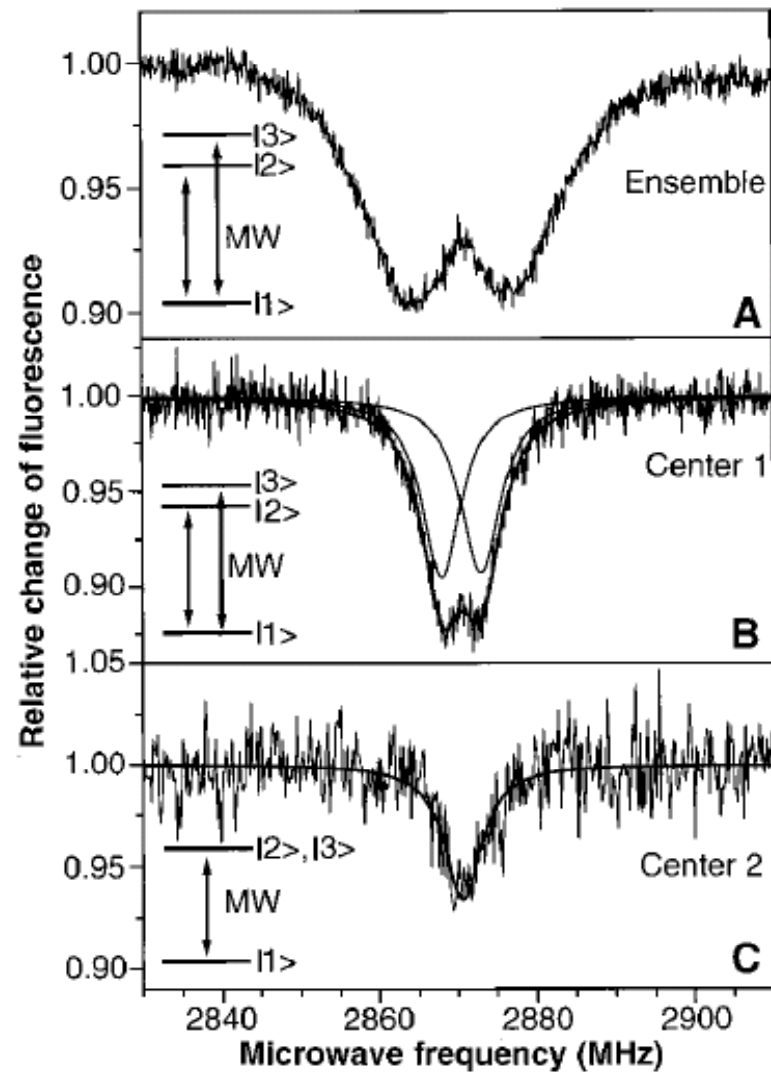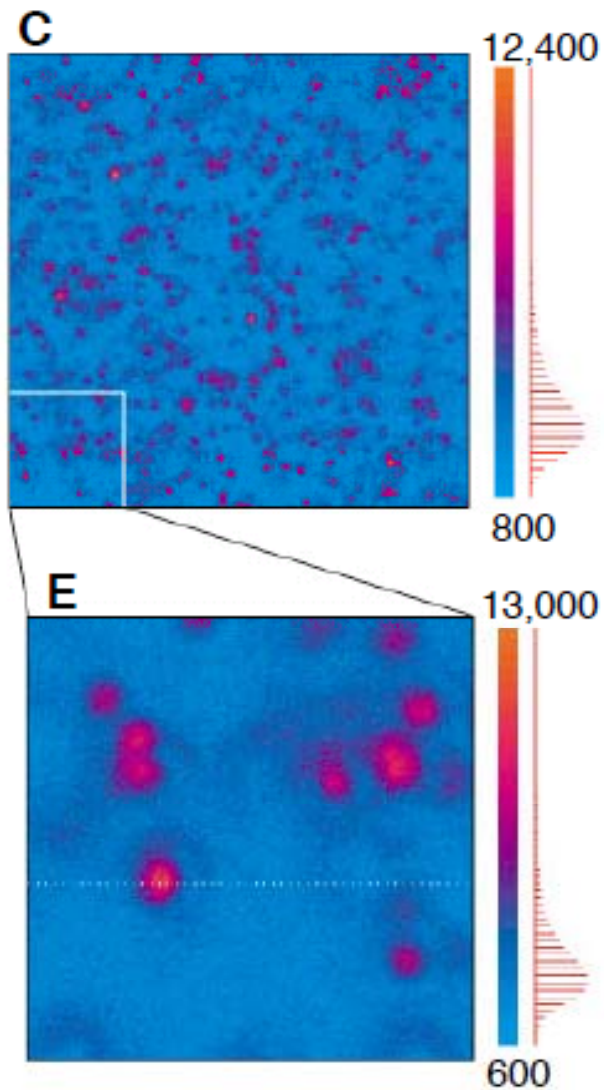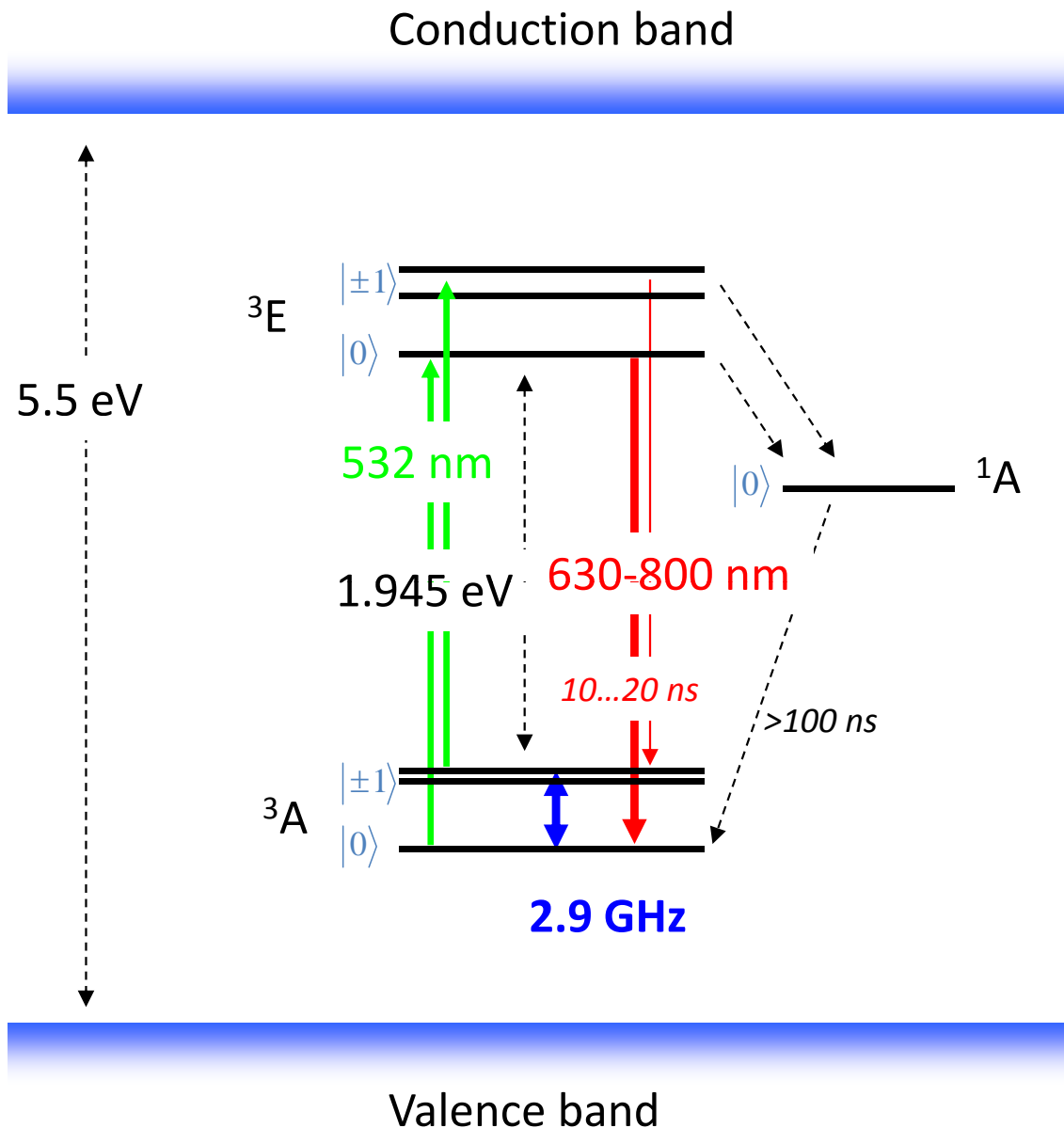
Spin Hamiltonian

$$\mathcal{H} = D\left(S_z^2 - \tfrac{1}{3}S^2\right) + \beta_e B \bar{\bar{g}}_e S + S\bar{\bar{A}}I$$

Zero field splitting
(2.87 GHz)

Electron Zeeman
(2.8 MHz/Gauss)

Hyperfine coupling to [14]N
(~2.2 MHz)
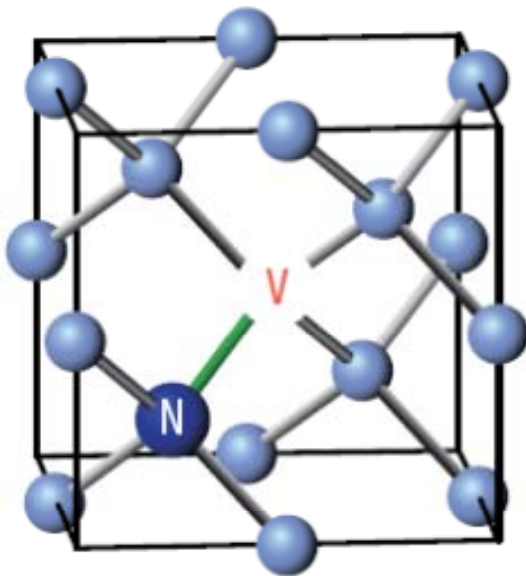
Spin Hamiltonian

$$\mathcal{H} = D\left(S_z^2 - \tfrac{1}{3}S^2\right) + \beta_e B \bar{\bar{g}}_e S + S \bar{\bar{A}} I$$

Zeeman
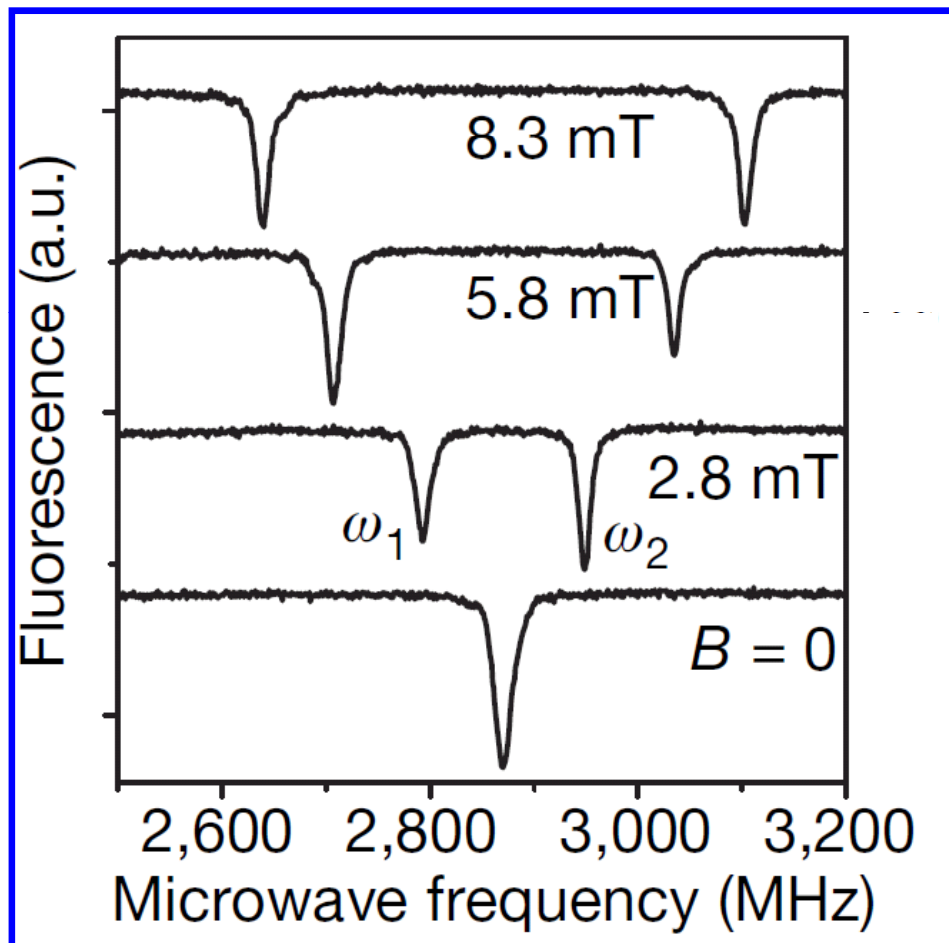
Hyperfine
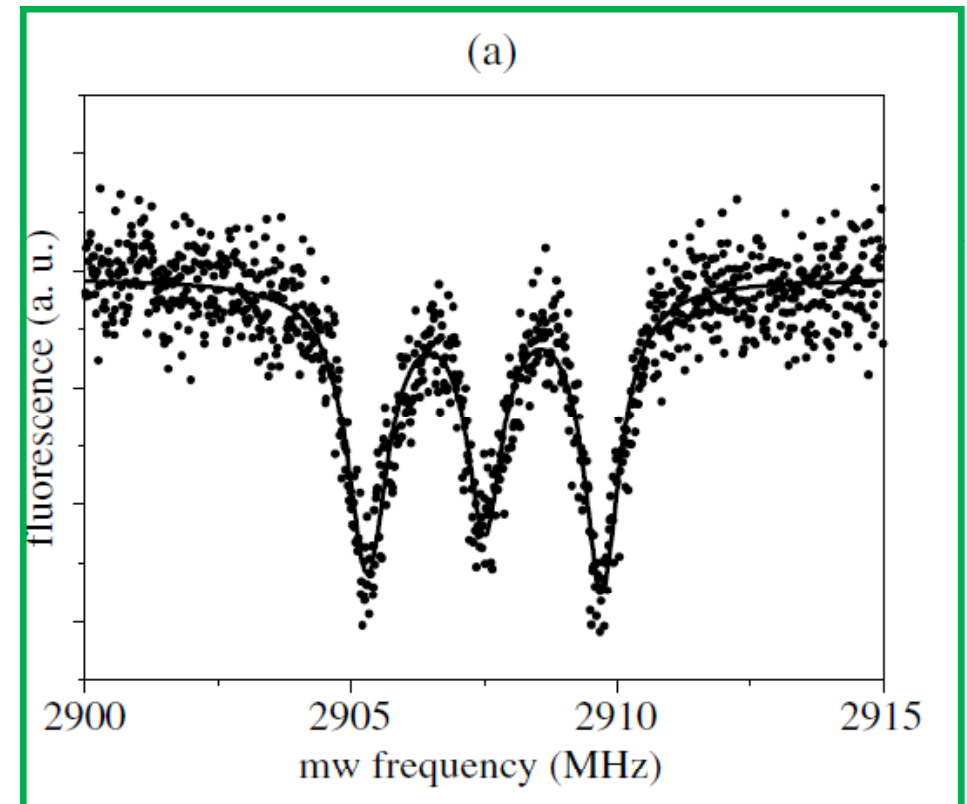
NV centers in diamond

Some properties:

- Single photon emitter

- Optically stable:
  No bleaching, no blinking

- High quantum yield ~70%

- Room temperature

- Long spin coherence times >1ms

- In nanodiamonds down to 5 nm

- Excellent chemical stability

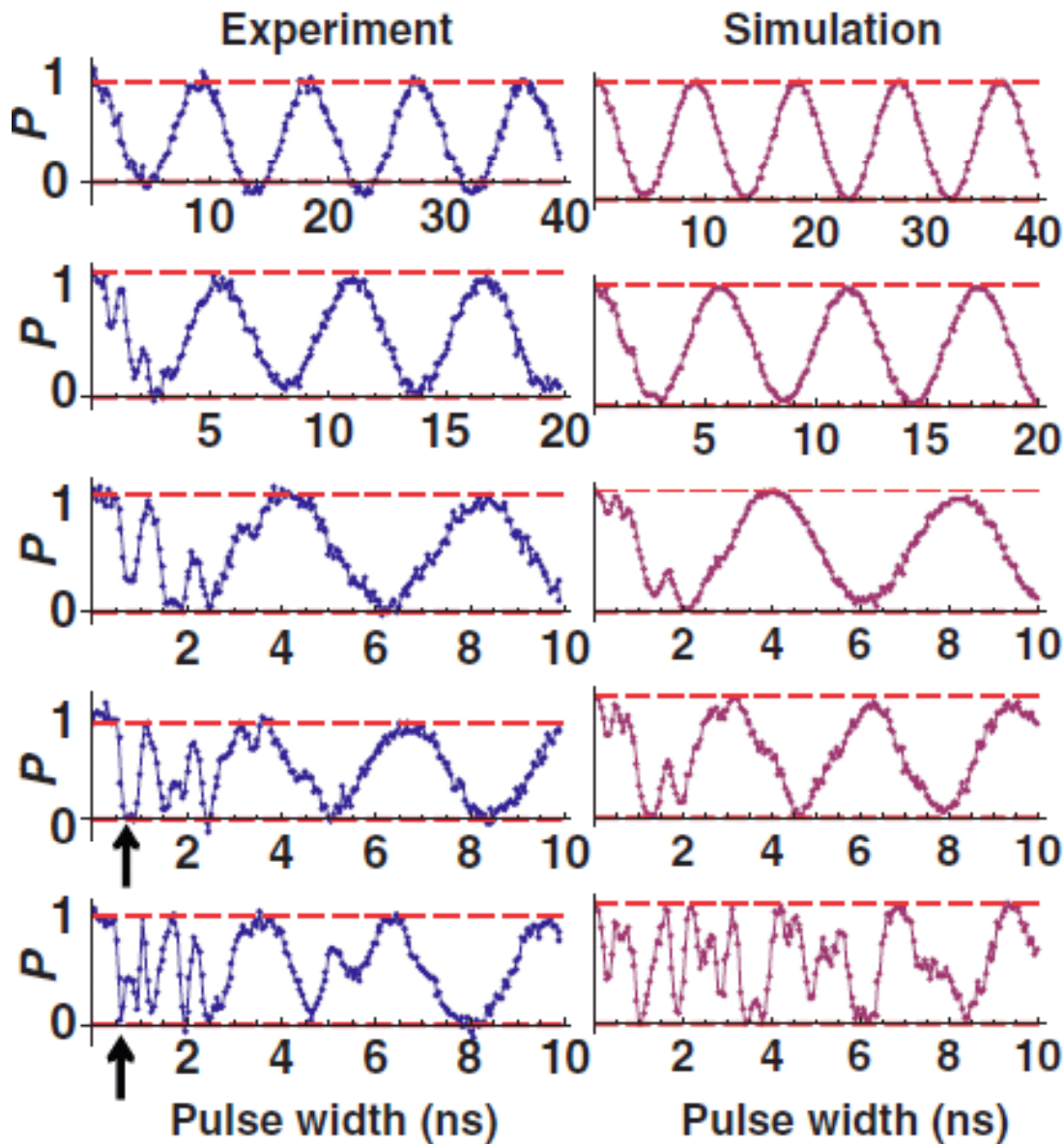- Non-toxic biomarkers

- Inexpensive!

- …
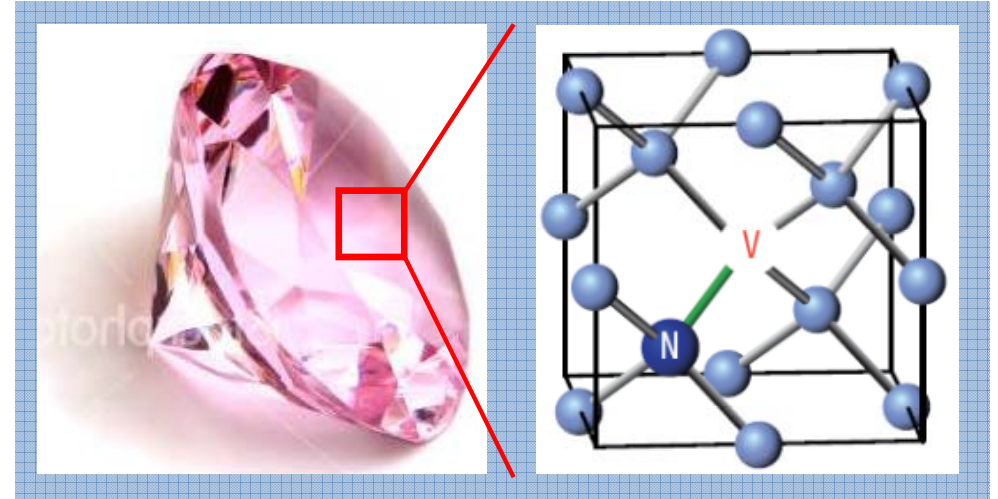
Nitrogen Vacancy defect in diamond

Fabrication – Ion implantation

NV centers implanted into single crystal diamond, then patterned with waveguide

Toyli, Nano Letters, 2010
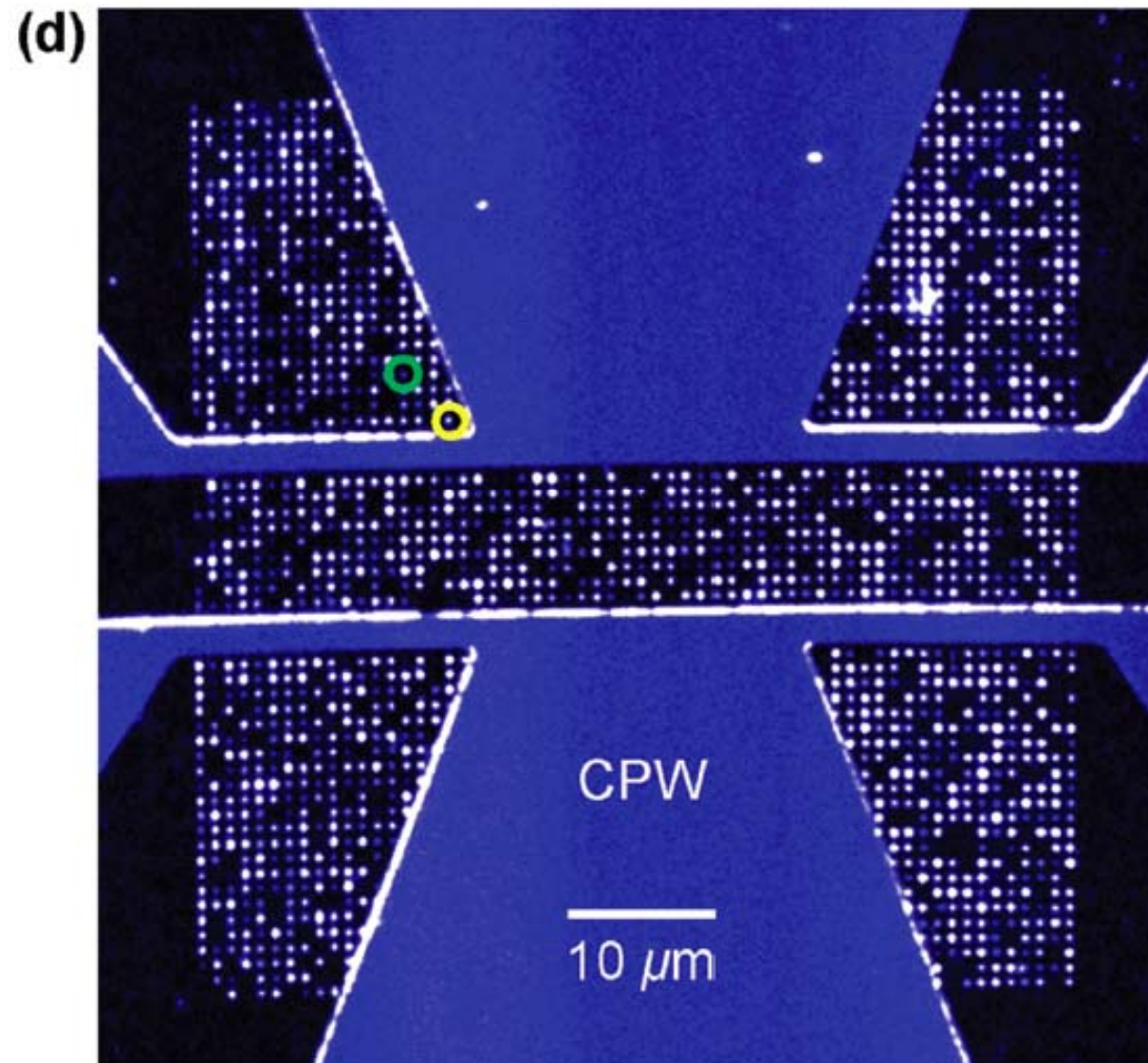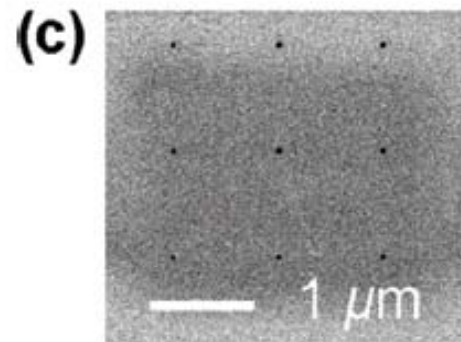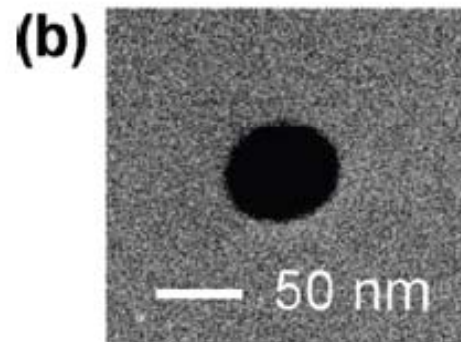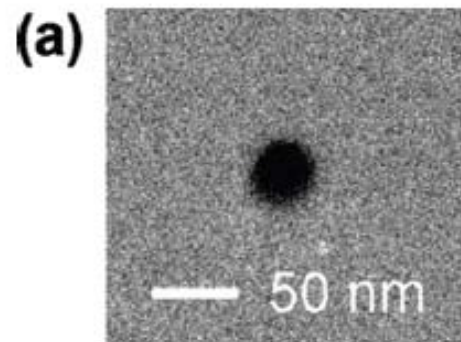
Rapid spin manipulation by waveguides

Rabi Oscillations

Spin inversion within ~ 1 ns

Single spins in diamond

Diamond nitrogen vacancy center (NV Center)
- Principles of Optically-detected magnetic resonance (ODMR)
- Initialization, manipulation, read-out of NV electron spin

→ Environment: Diamond host material

Applications

Spin environment

Nuclear spins

- ^{14}NV nuclear spin (I=1)
- ^{13}C spins (I=½)
  1.03% natural abundance
  - First shell: 3x dangling bonds
  - Second, third, … shell
  - Distant: "Classical" spin bath

- …
- Surface spins (adsorbates)

Electron spins

- Nearby **N defect** electron spins (S=1/2) ("P$_1$ or C centers")
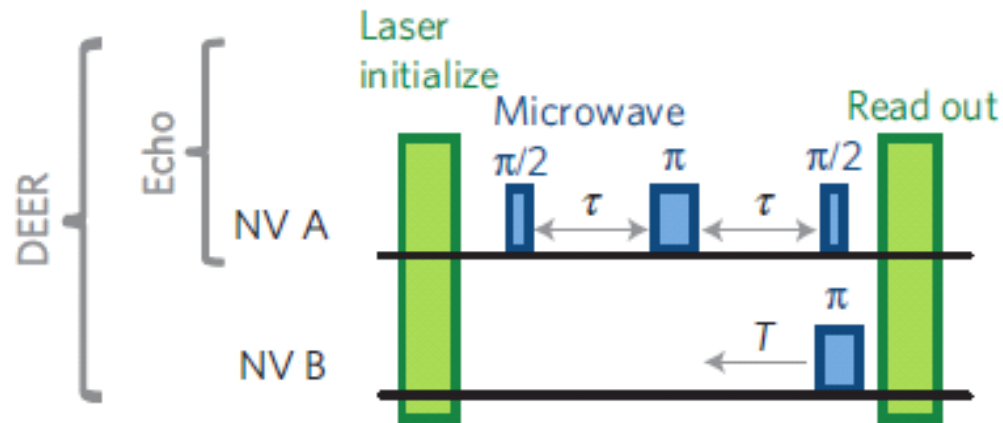- Nearby other **NV center** (S=1)
- …
- Surface spins (electronic, nuclear)
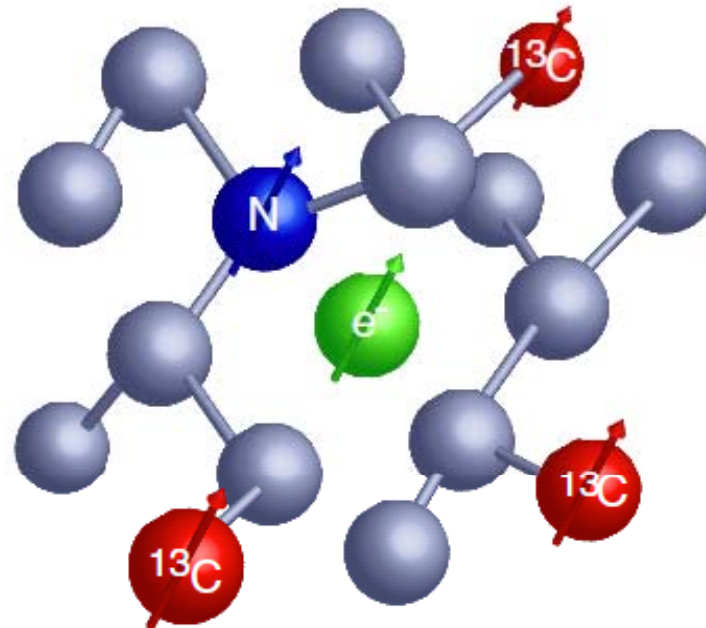
Other electronic spins

Nearby N defect with S = ½ ("P1 center")

Gaebel, Nature Physics, 2006
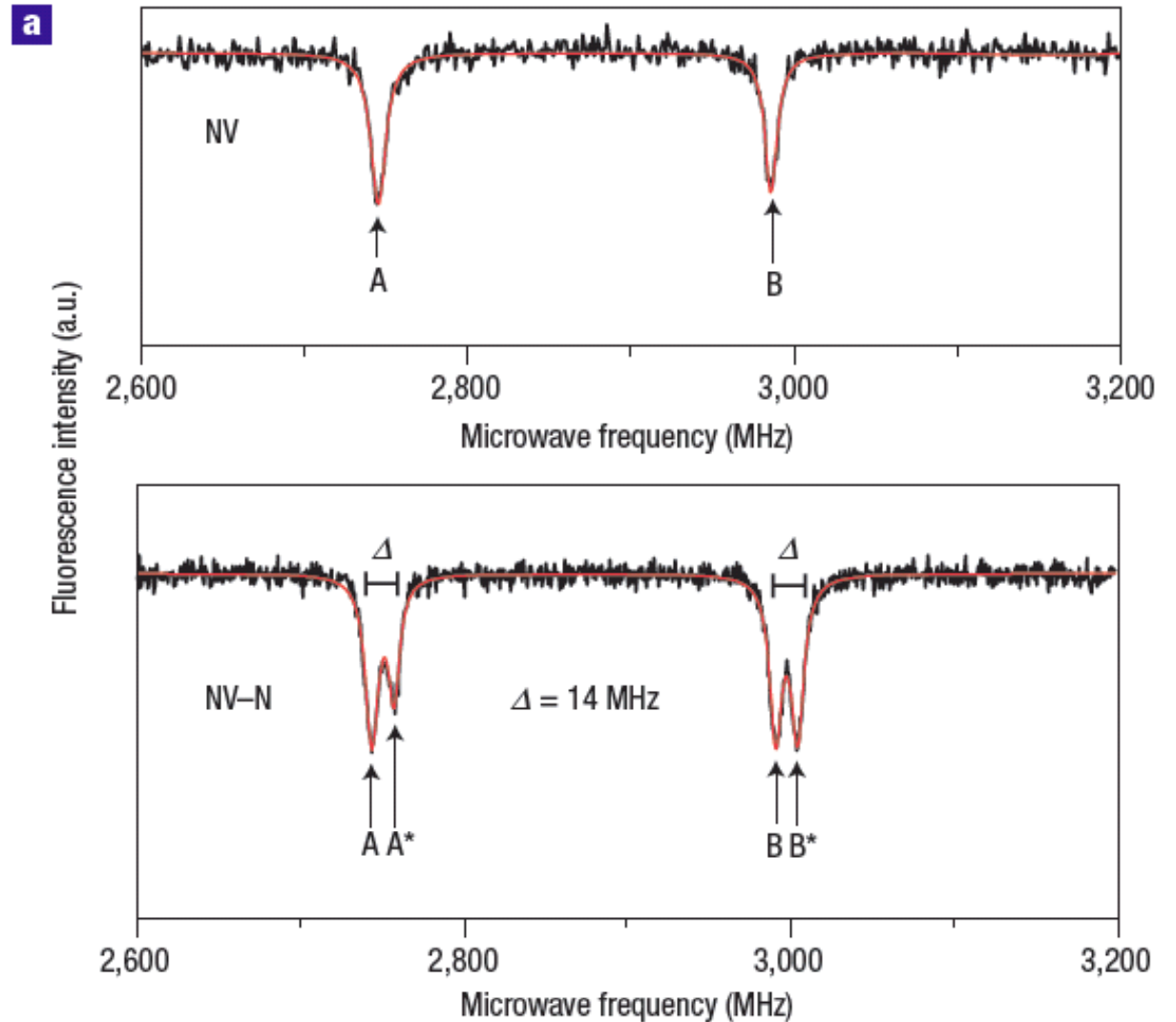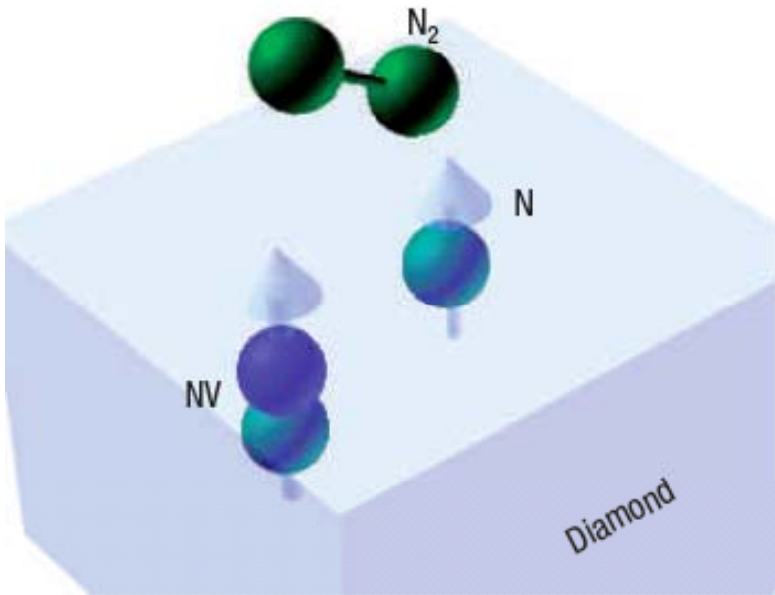
Coupling between two NV centers

Neumann, Nature Physics, 2010
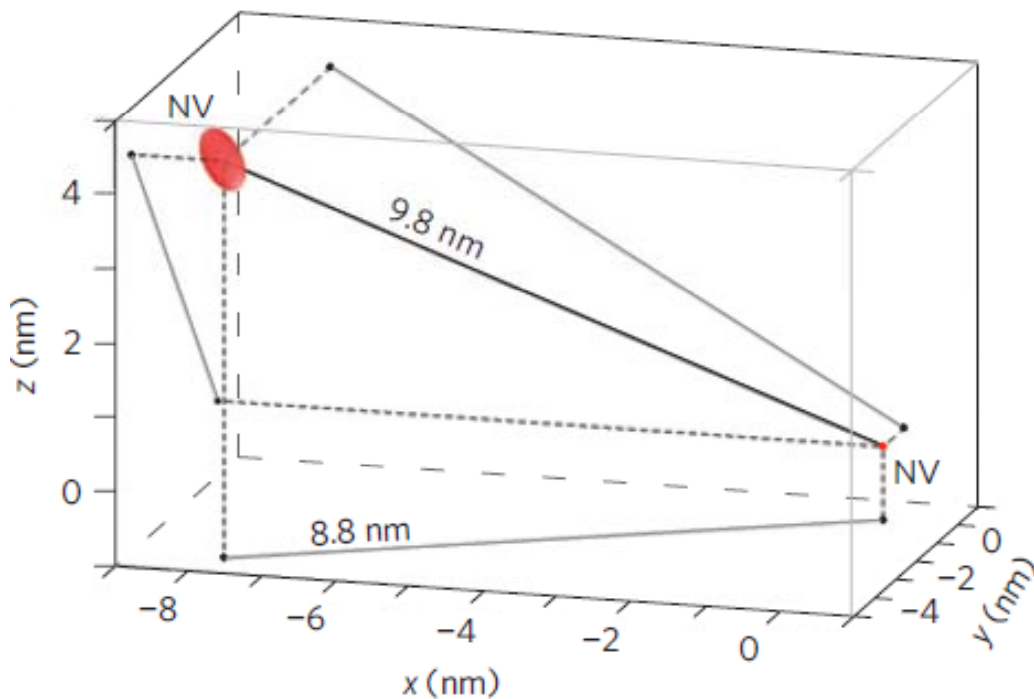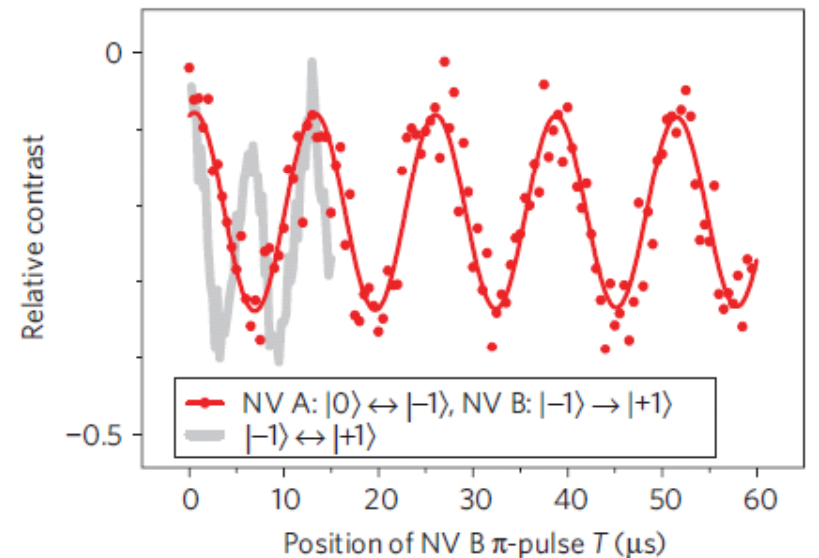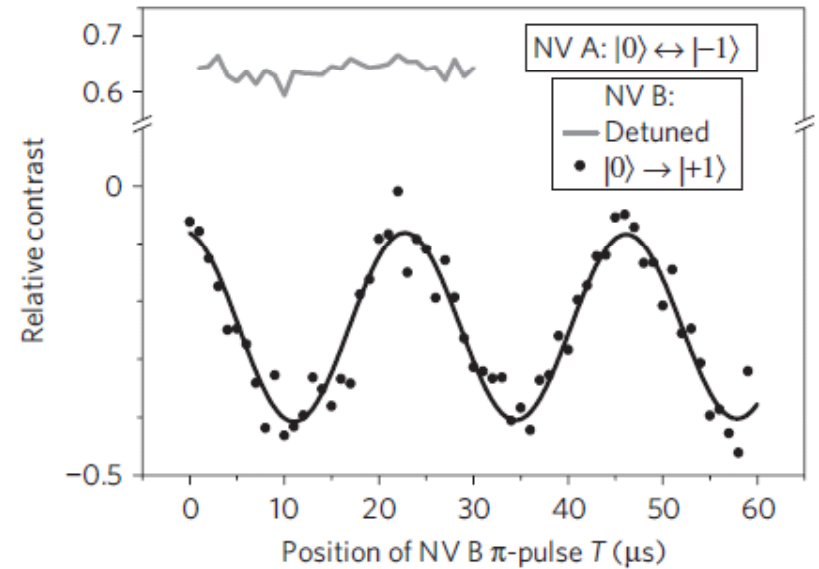
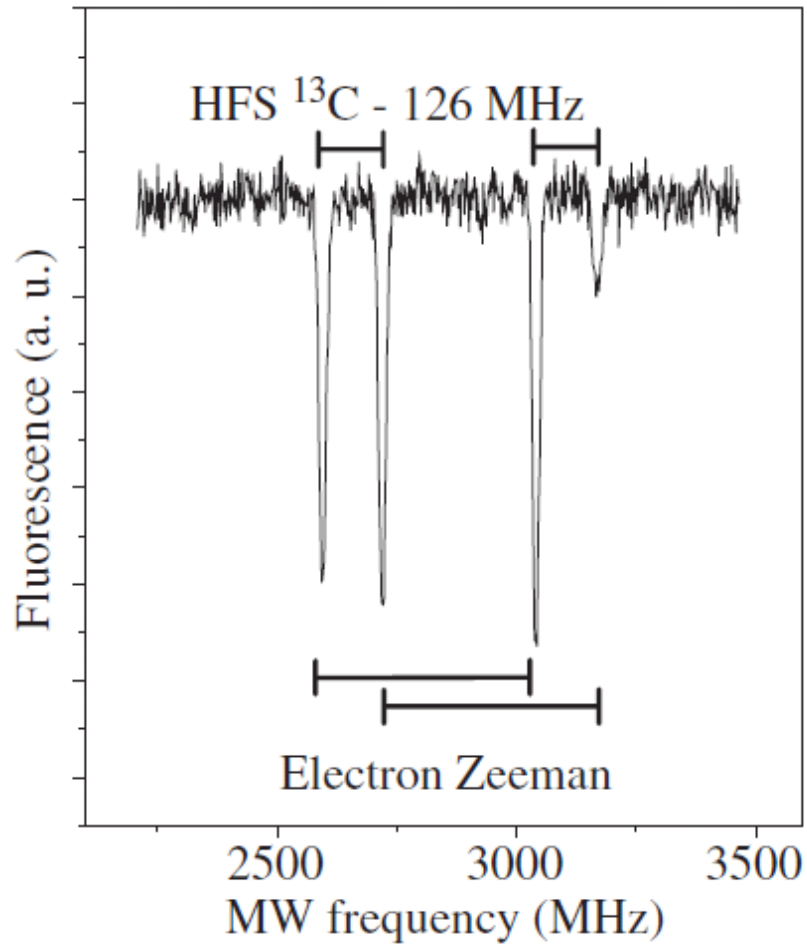# The ^{13}C nuclear spin environment
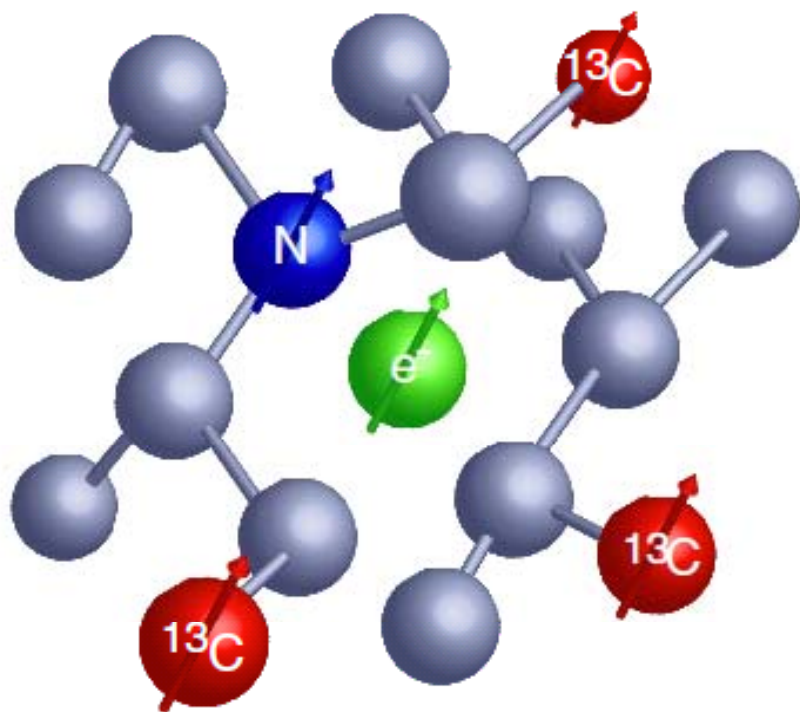
Near ^{13}C spins – resolved lines

Intermediate ^{13}C spins – lines not resolved, but still moderate hyperfine coupling

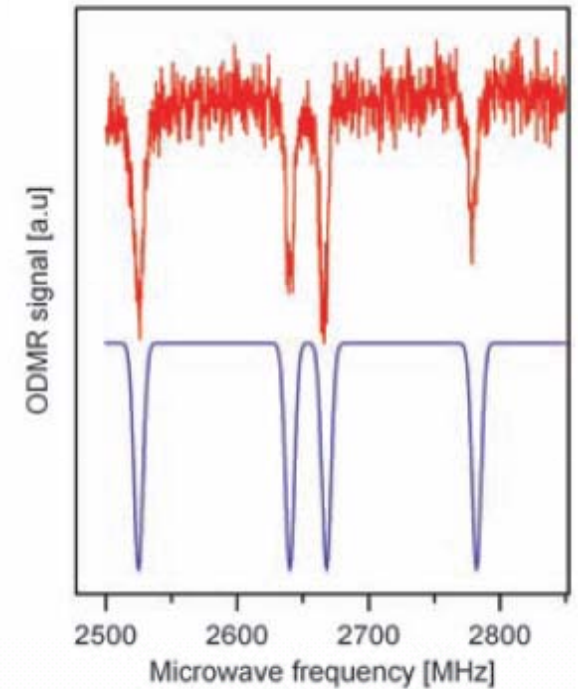**Distant ^{13}C spins** – very weak hyperfine coupling ("classical ensemble")

Specific nearby ¹³C

Two qubits: NV + ¹³C

Three qubits: NV + ¹³C + ¹³C

Dutt, Science, 2007

Repetitive readout

Store and Readout NV spin state in nearby ^{13}C nucleus

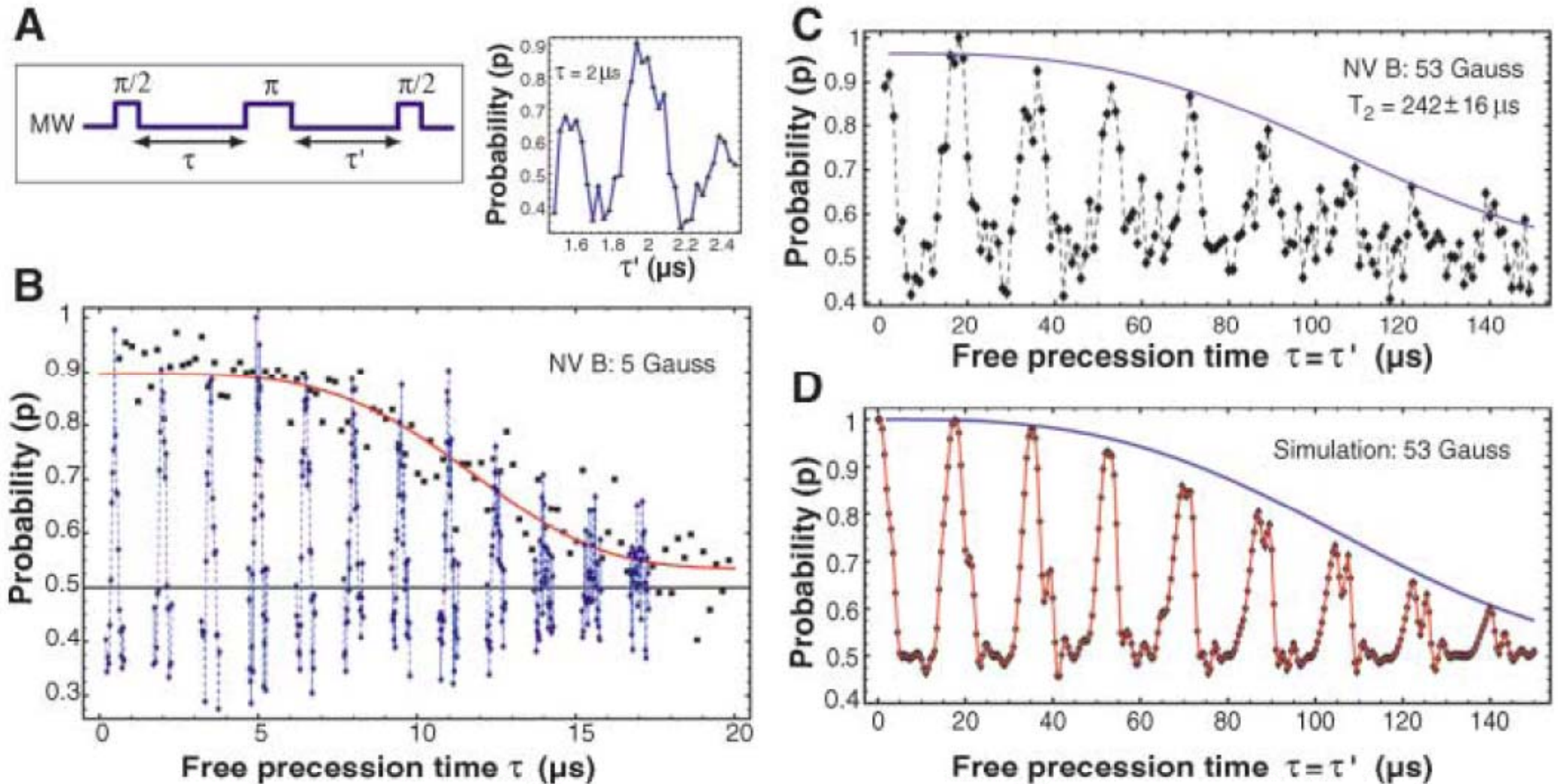init   calculation   store   readout n

Jiang, Science, 2009
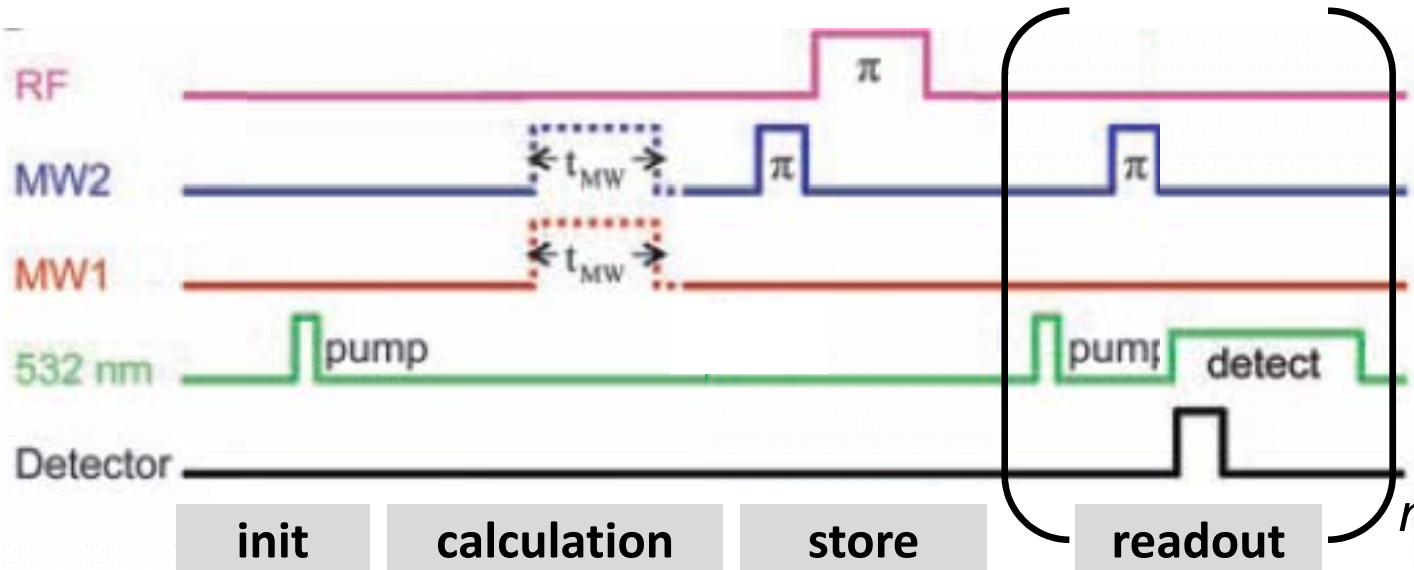
Example:
Rabi oscillation
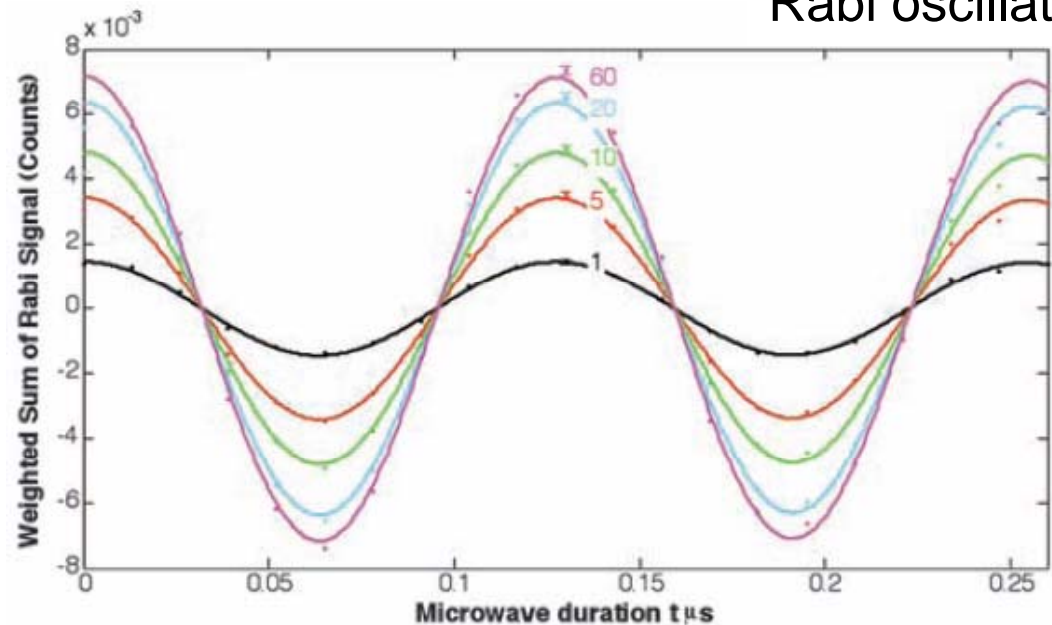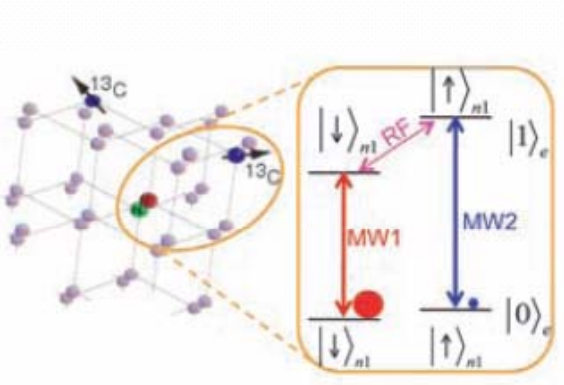
Distant ^{13}C spin bath

Periodic "revivals" of spin echo with ^{13}C Larmor frequency

Childress, Science, 2006

Eliminating ¹³C nuclear spin bath

The materials scientists' way ...

¹³C content	Spin coherence time T_2
20.7%	0.010 ms
8.4 %	0.12 ms
1.1 % (natural)	0.65 ms
0.4%	1.8 ms

Balasubramanian, Nature Materials, 2009
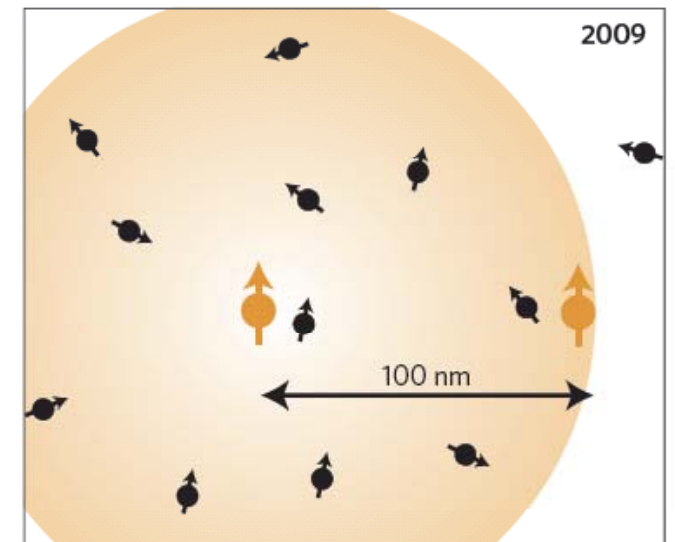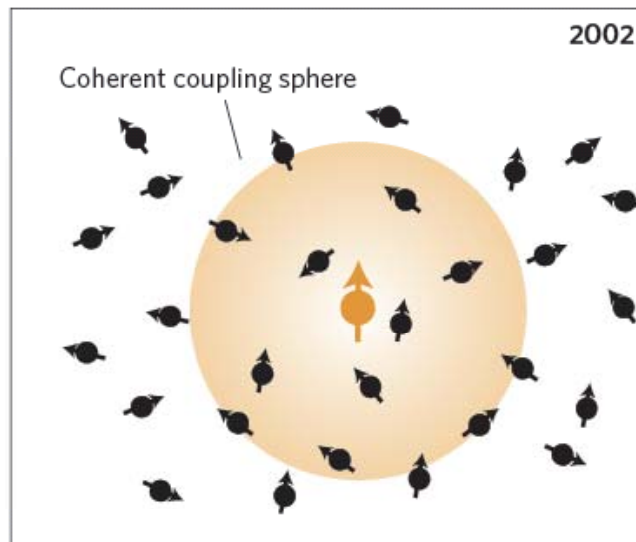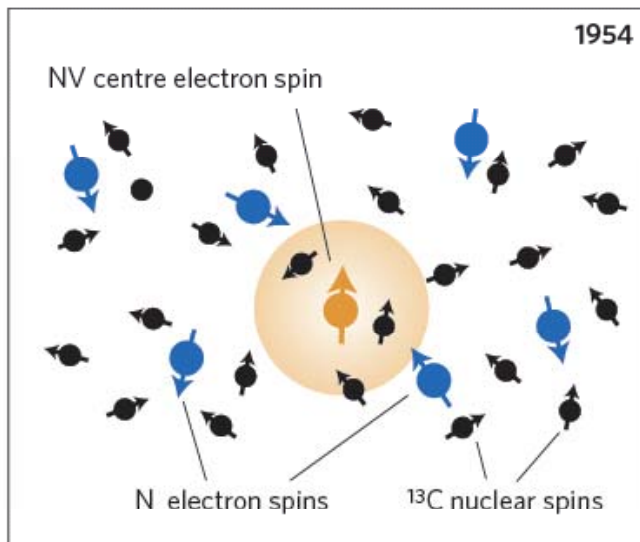
Eliminating ^{13}C nuclear spin bath

... the spectroscopists way

Multi-pulse decoupling
(also "dynamical decoupling")
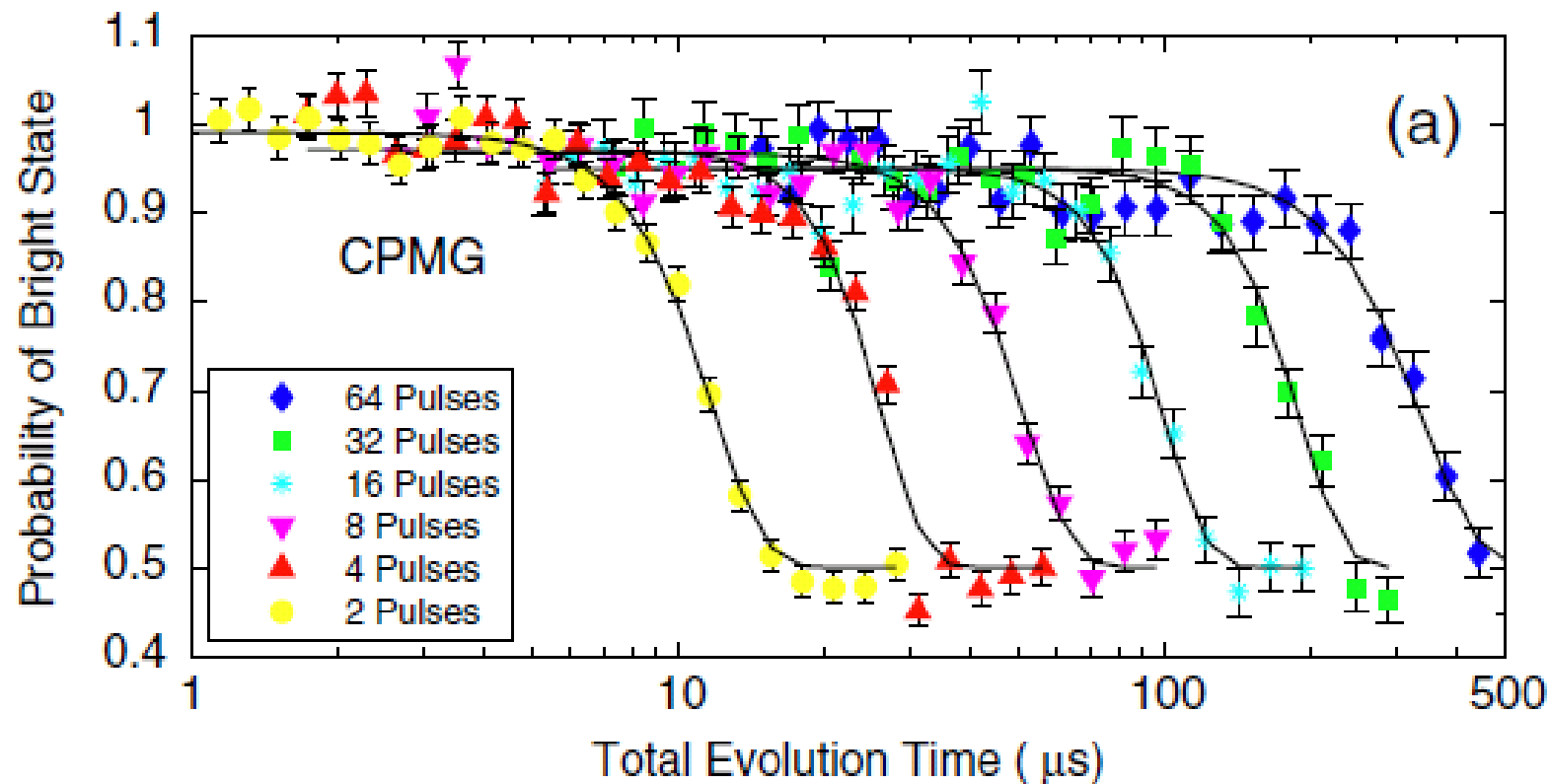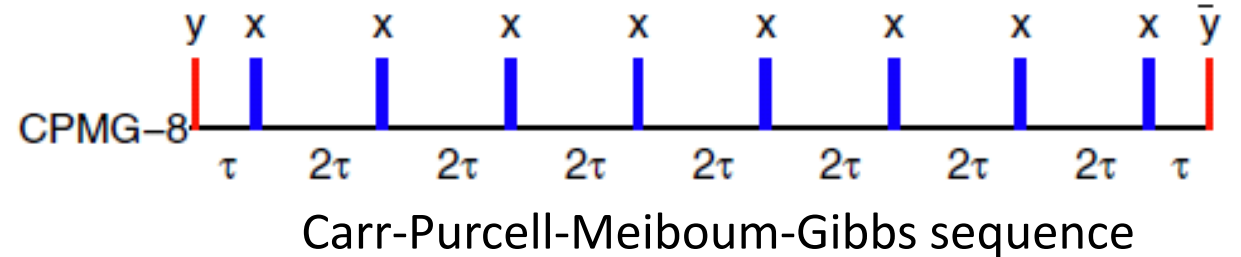
Carr-Purcell-Meiboum-Gibbs sequence

Single spins in diamond

Diamond nitrogen vacancy center (NV Center)
- Principles of Optically-detected magnetic resonance (ODMR)
- Initialization, manipulation, read-out of NV electron spin

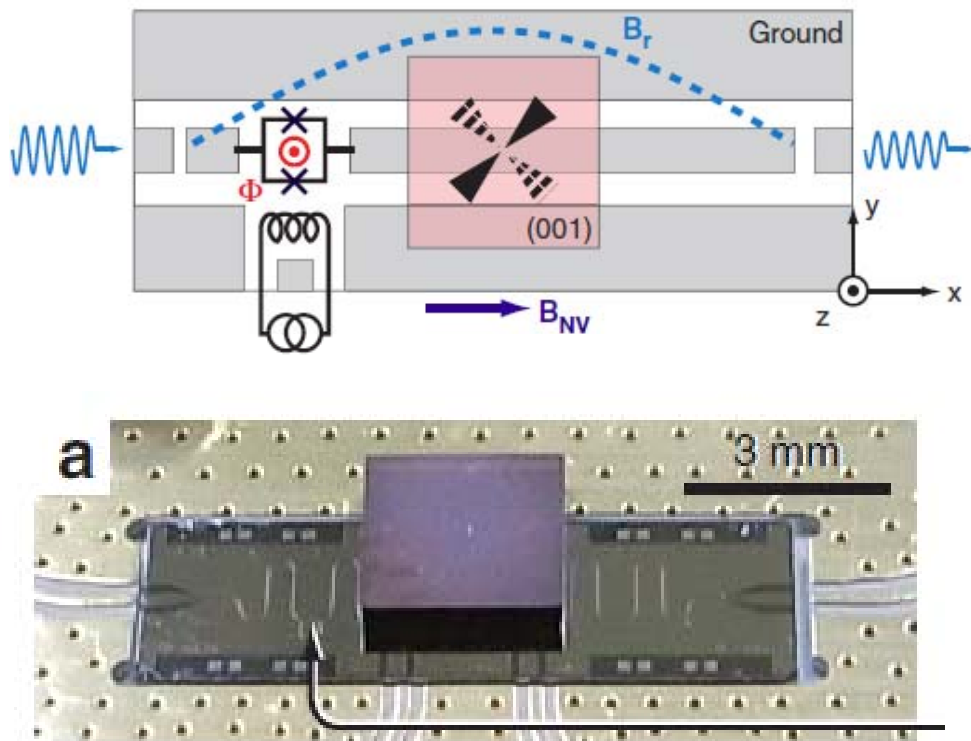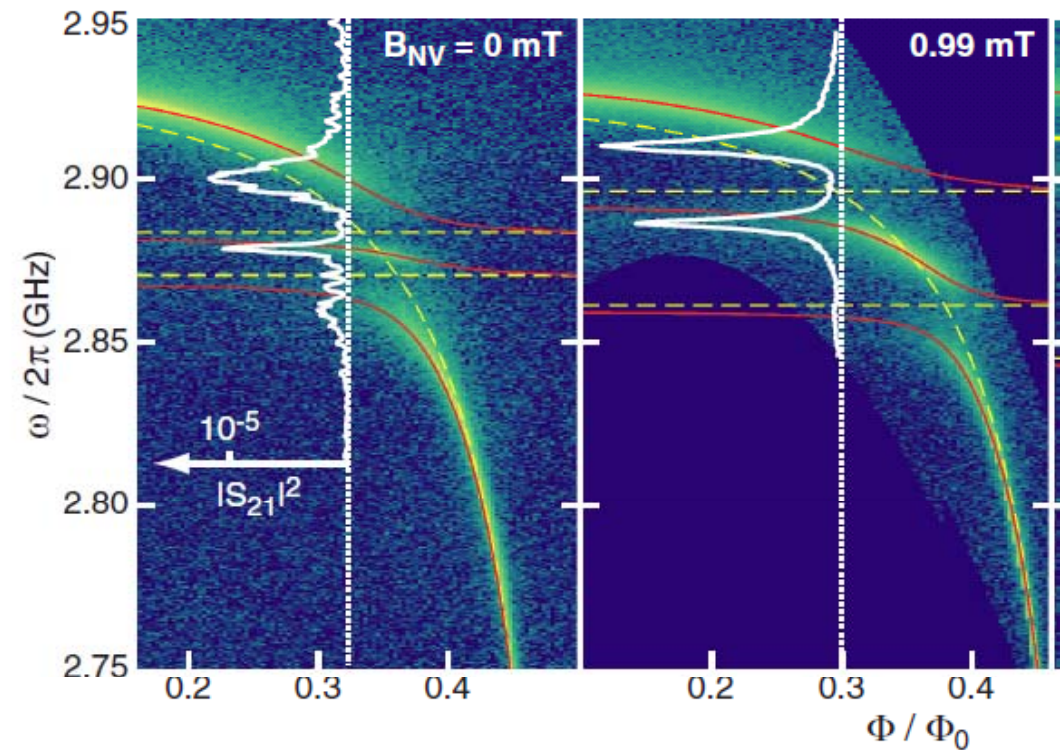Environment: Diamond host material

➡ Applications

Hybrid implementations

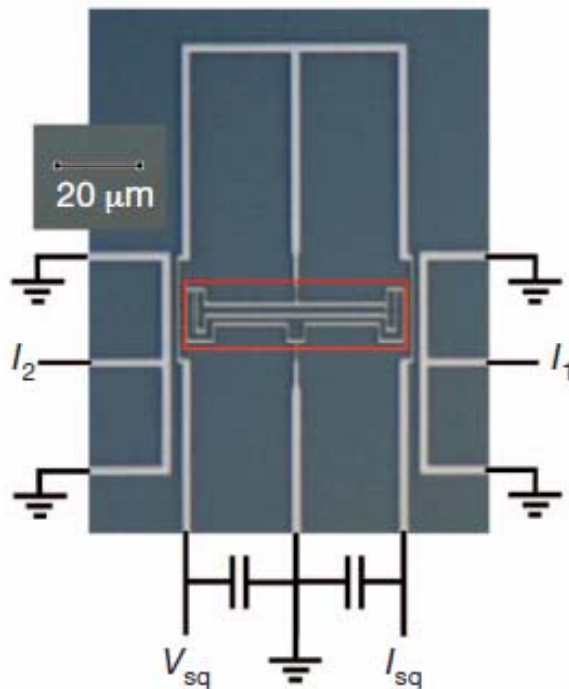## NV centers to superconducting microwave resonator

Arrangement

Transmission vs. Frequency

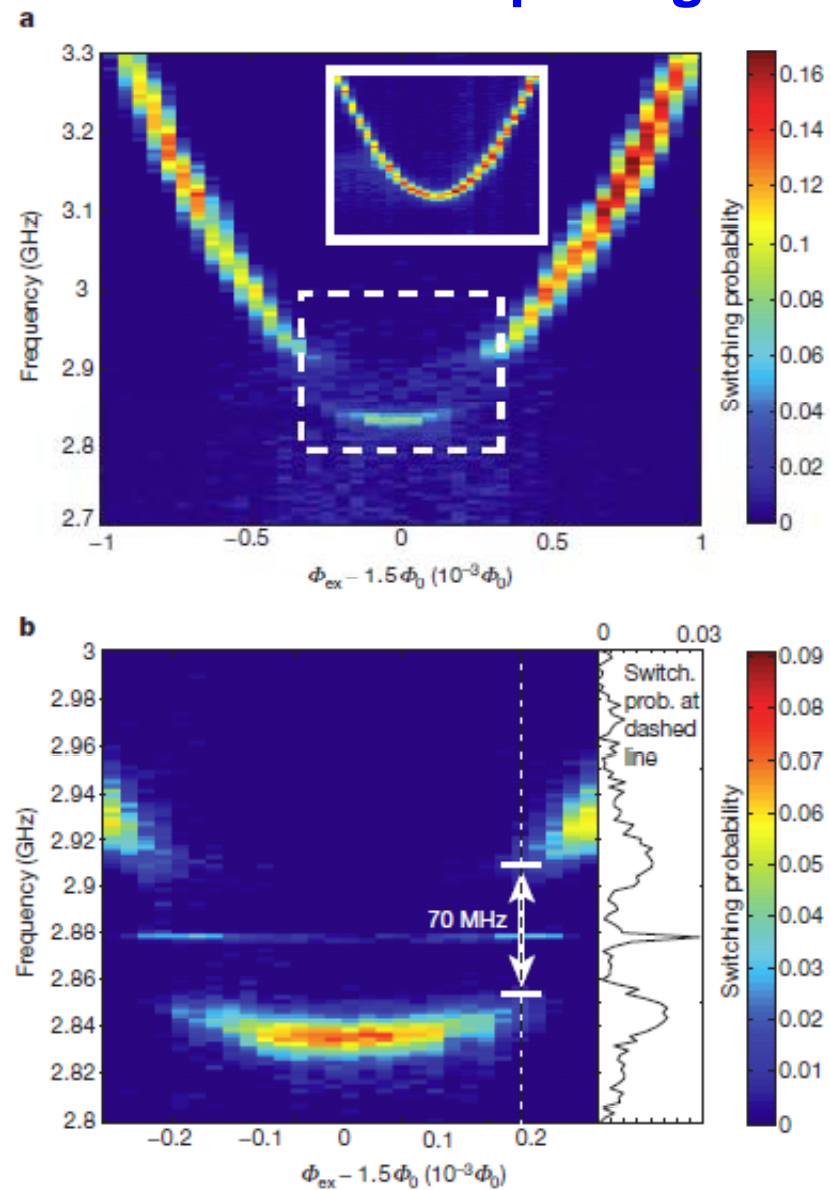
Kubo, PRL, 2010

Flux qubit

Vacuum Rabi splitting

Arrangement

Semba, Nature, 2011
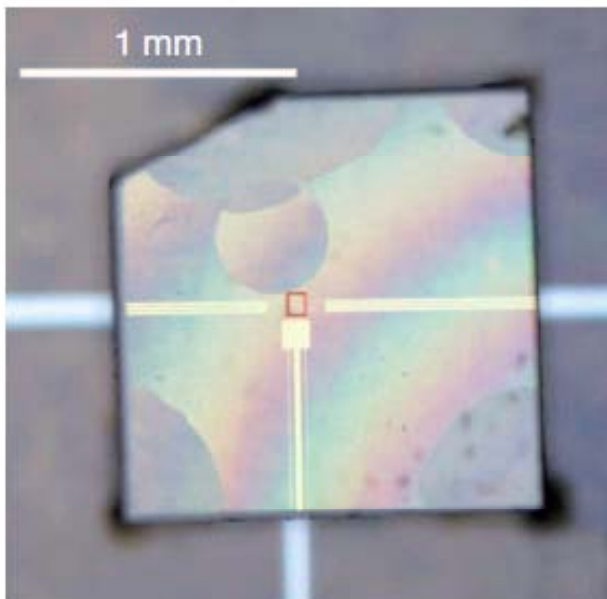
Nanomechanical resonators

Arcizet, Nature Physics, 2011
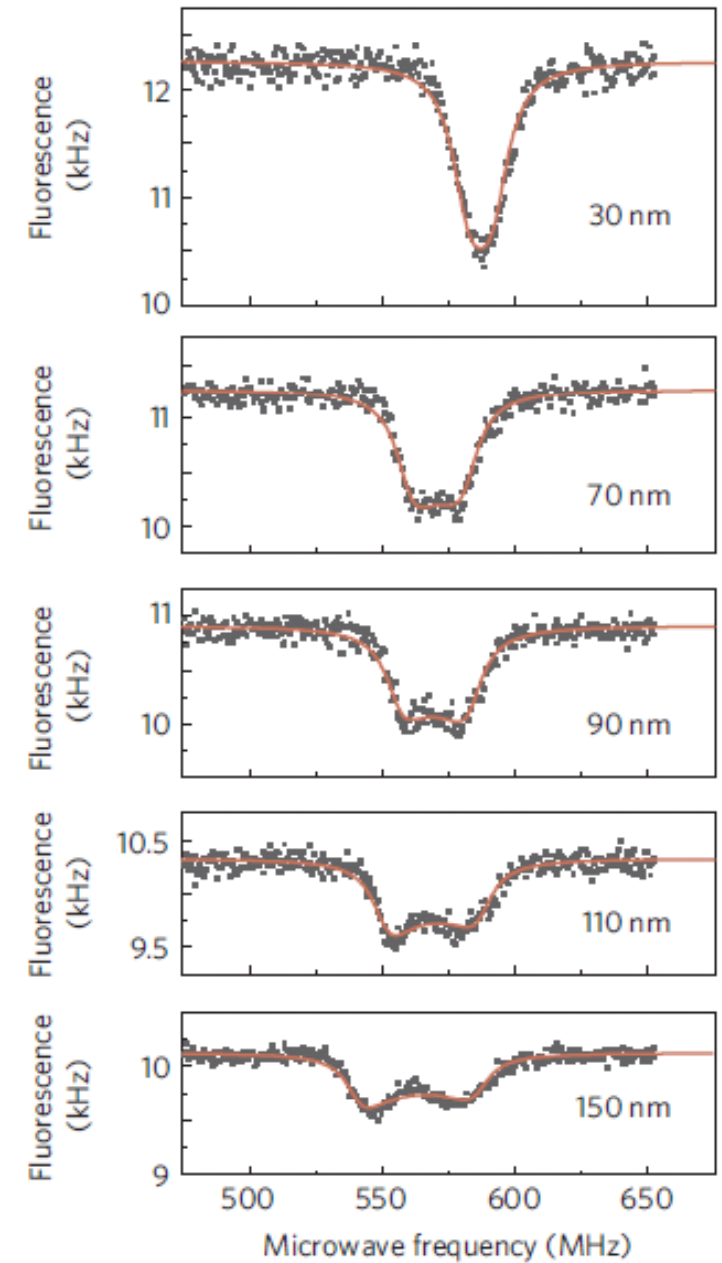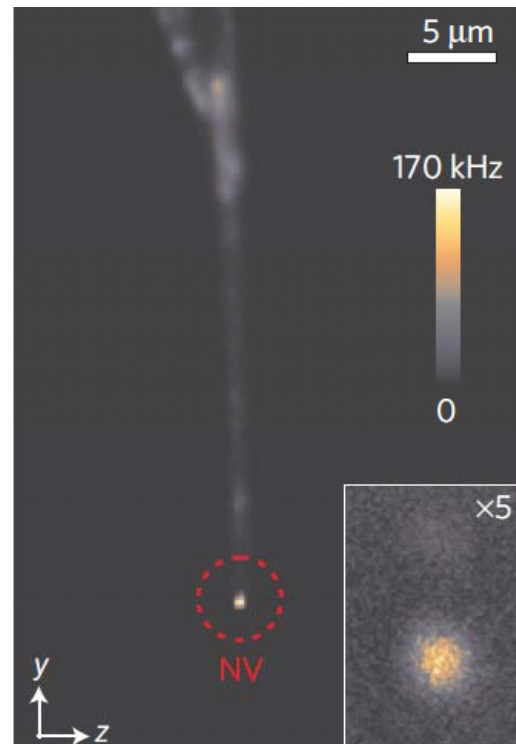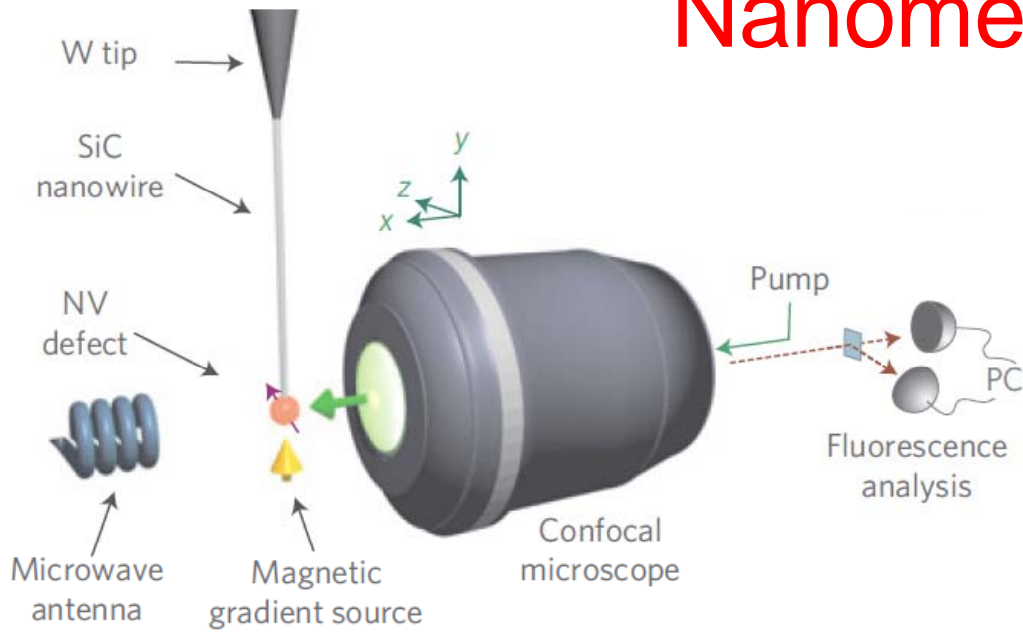
Application in nanoscale magnetic imaging

Degen, Appl. Phys. Lett, 2008
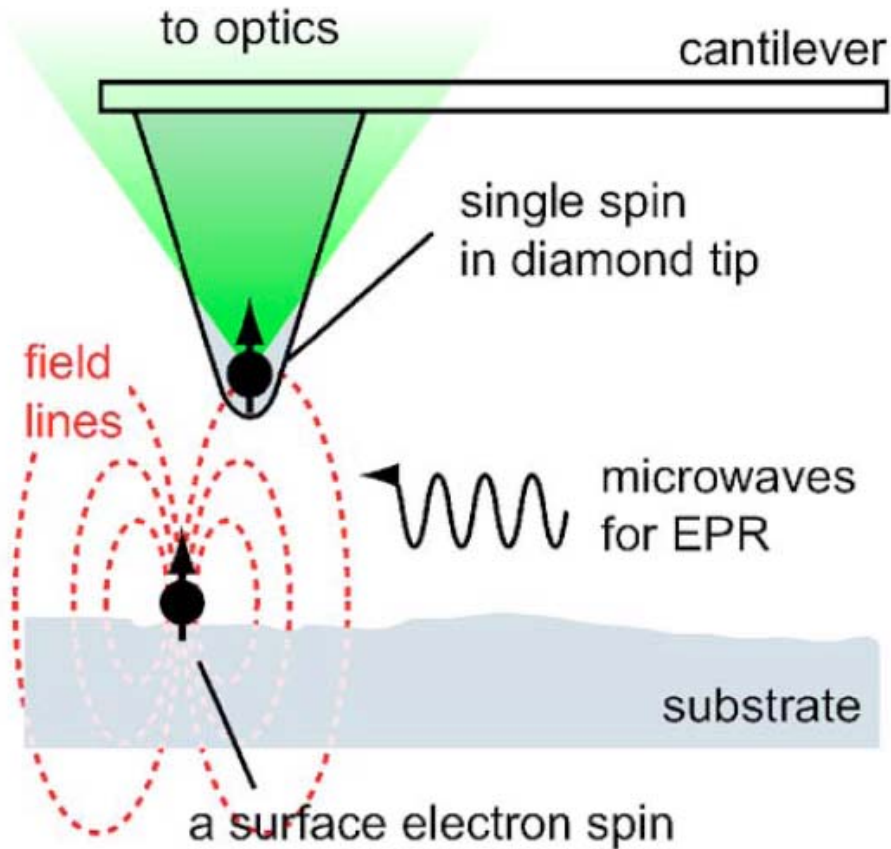
Measure nanoscale magnetic fields from:

- Single electron spins
- Nuclear spins in (bio)molecules
- Superconductors
- Magnetic nanostructures
- Quantized currents in mesoscopics

Disk drive (Rondin, arXiv, 2011)