Magnetic Resonance in Quantum Information

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Content

Features of (nuclear) magnetic resonance

Brief History of NMR

Example 1:

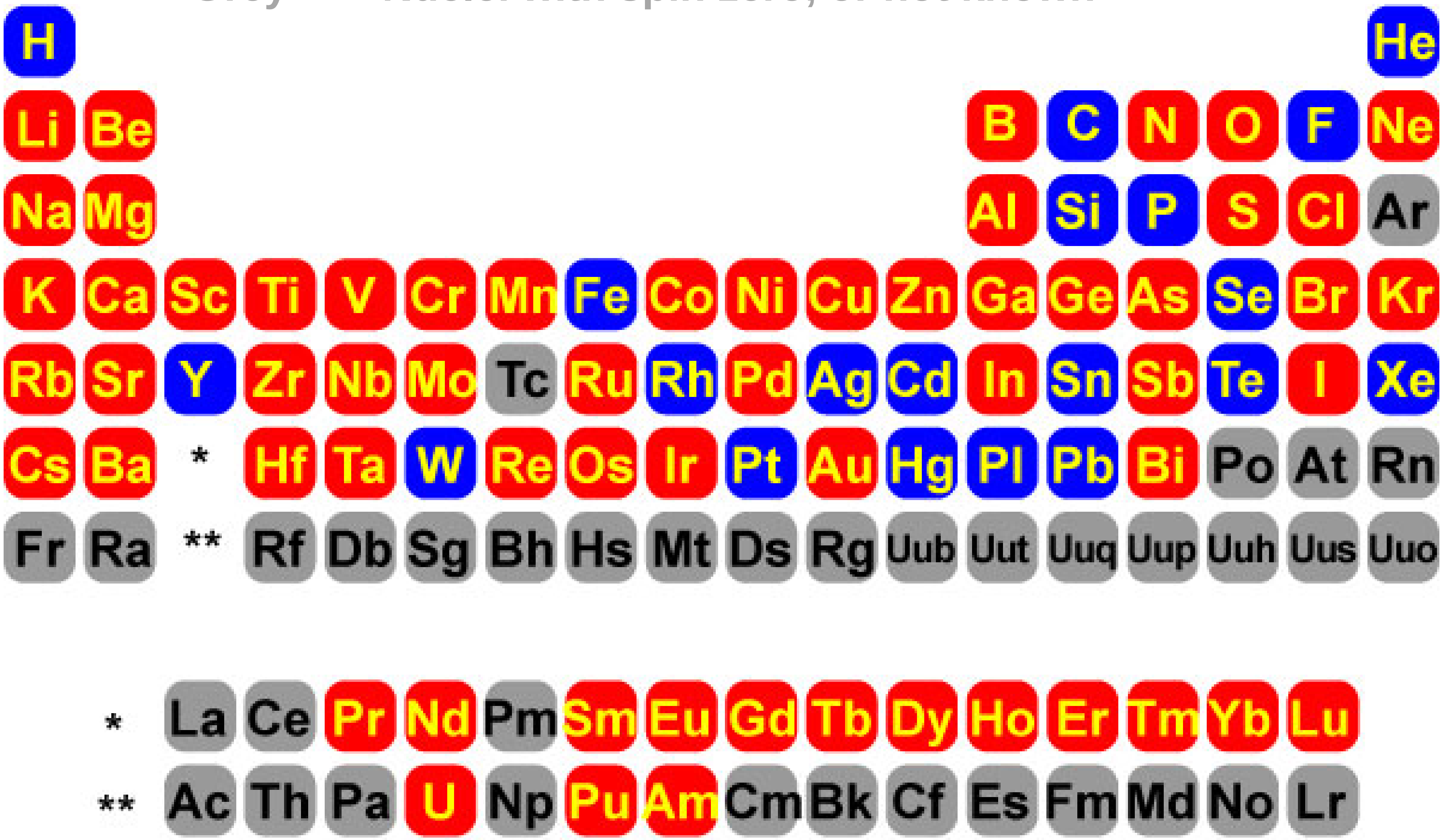
Liquid-state NMR (=> Factoring of 15)

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

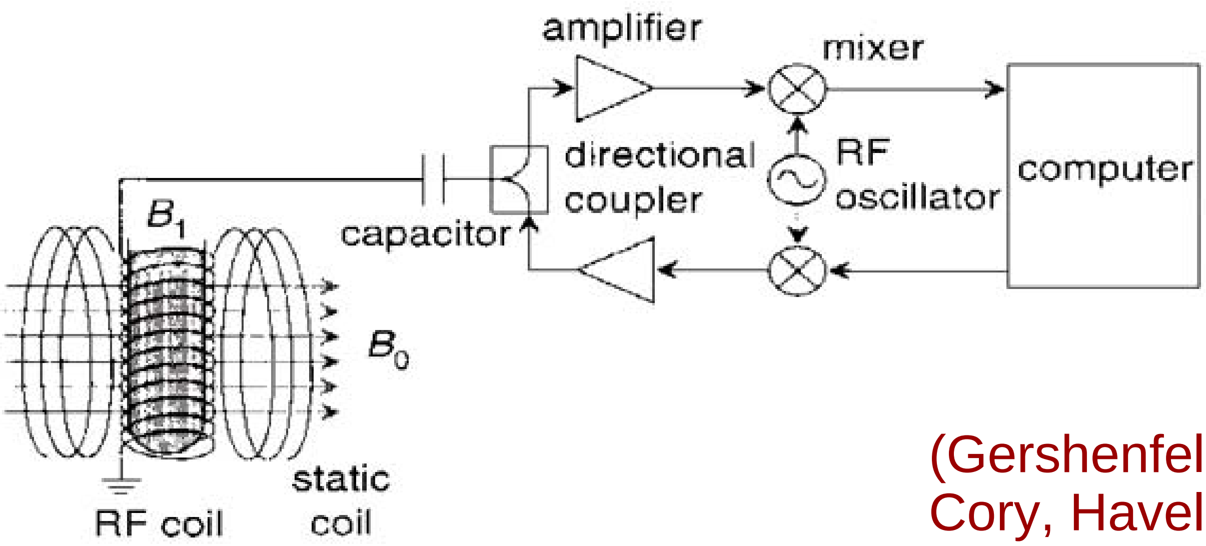


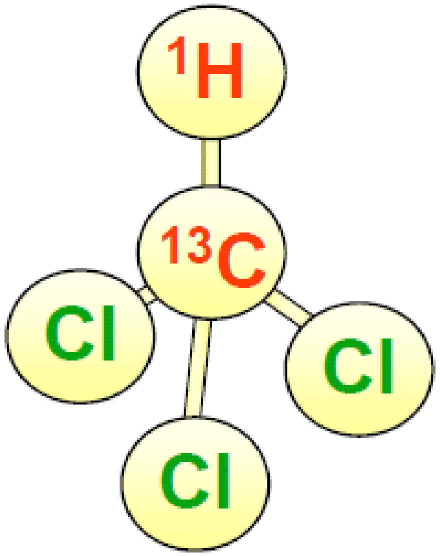
Time and Energy scales in NMR & EPR

	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)	$\sim 10^{-5}$	~1%
• Spin relaxation time T_1	$0.1 \ldots 10^{5}$ s	$10^{-9} \ldots 1$ s
• Spin coherence time T_2	~1…100μs (solids) ~10ms…10s (liquids)	$10^{-9} \ldots 10^{-3}$ 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





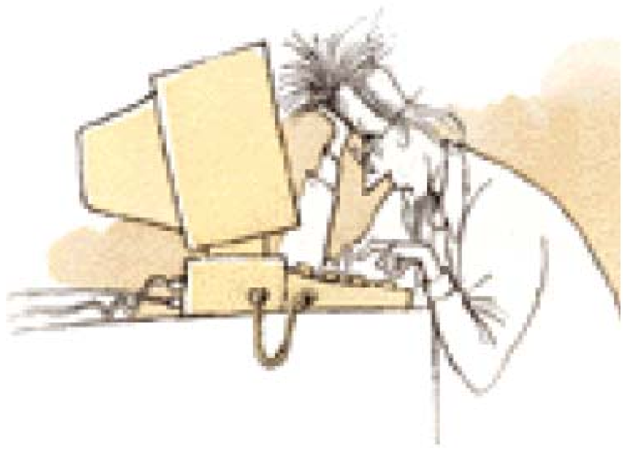
(Gershenfeld & Chuang 1997,
Cory, Havel & Fahmi 1997)

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

Molecule Selection

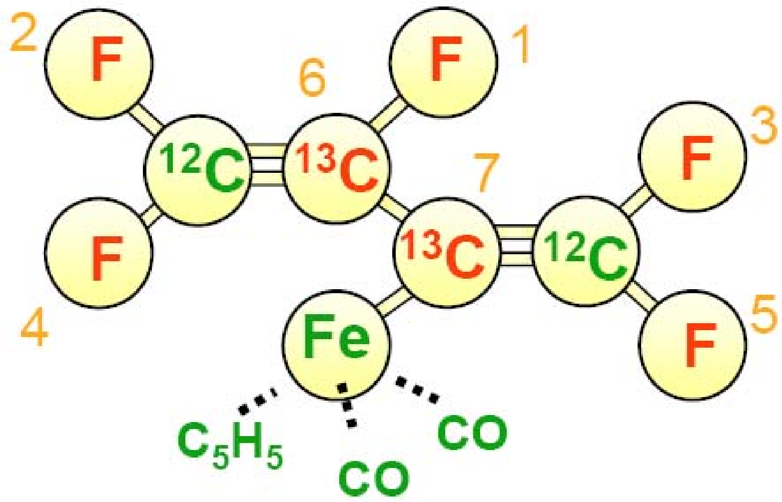
Summary: Pro’s & Con’s

=> “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

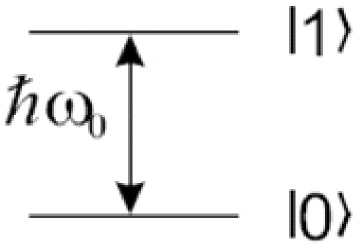
Survey of NMR quantum computing

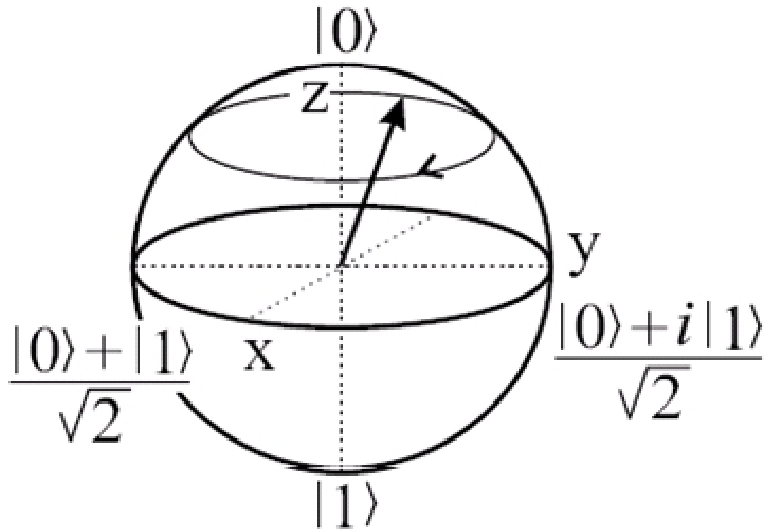
- ➡ Principles of NMR QC
- Molecule Selection
- Summary: Pros & Cons

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

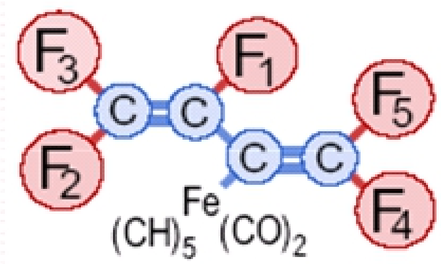
energy: $H_0 = -\vec{M}\cdot\vec{B}_0$

gyromagnetic (g-)factor: γ

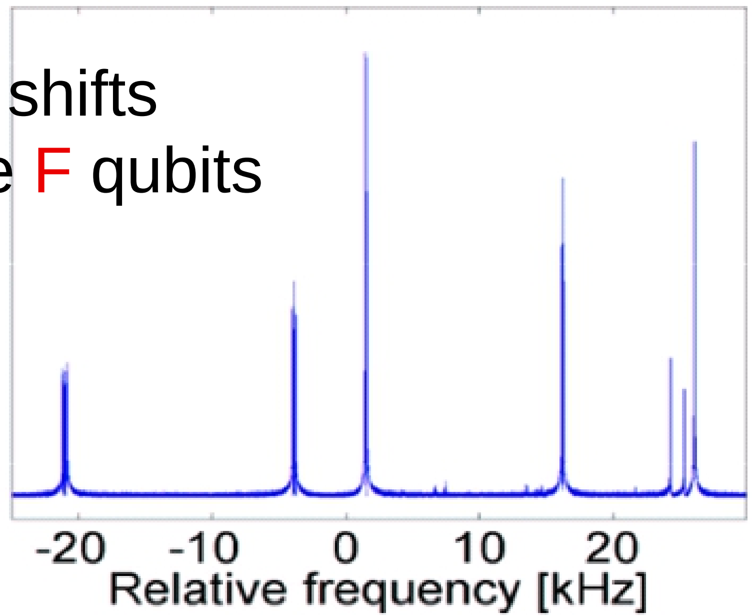
Nuclear spin Hamiltonian
Multiple spins

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

σz σx σy

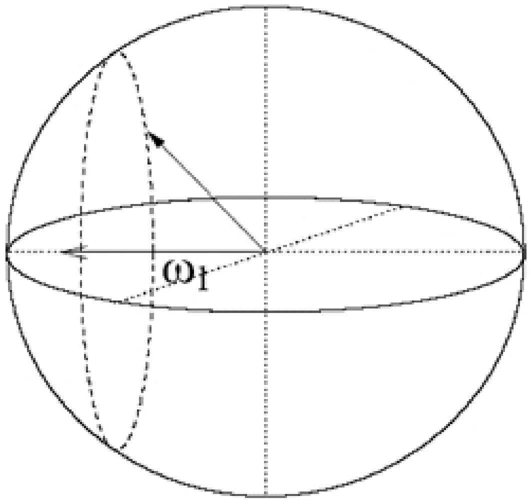
$$\mathcal{H} = -\hbar\,\omega_0\, I_z - \hbar\omega_1 \left[\cos(\omega_{rf} t + \phi) I_x + \sin(\omega_{rf} t + \phi) I_y\right]$$

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

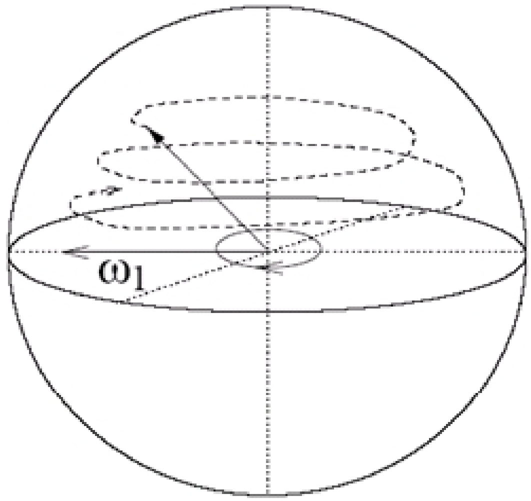
$$\mathcal{H}^{rot} = -\hbar\,(\omega_0 - \omega_{rf})\, I_z - \hbar\omega_1 \left[\cos\phi\, I_x + \sin\phi\, I_y\right]$$

rotating wave approximation

typical strength I_x, I_y : up to 100 kHz



Rotating frame



Lab frame

Nuclear spin Hamiltonian

Coupled spins

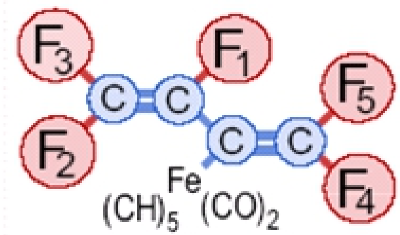
J>0: antiferro mag.

J<0: ferro-mag.

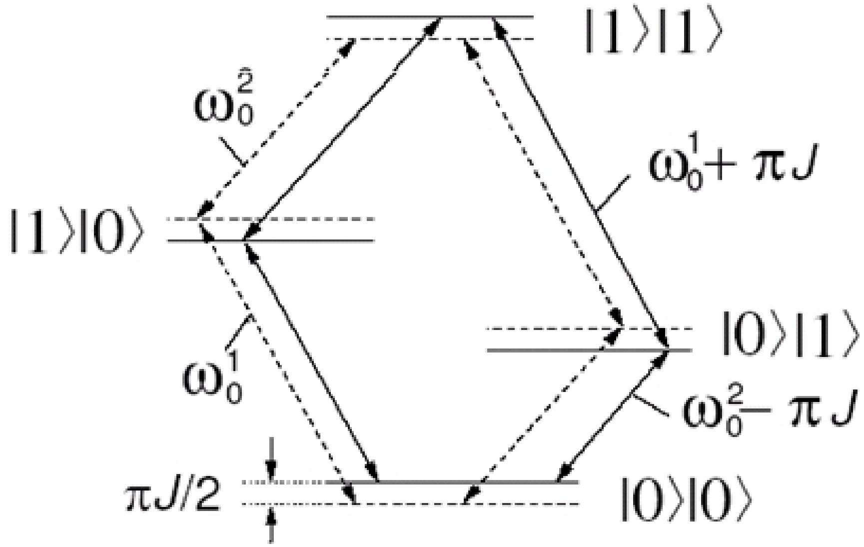
coupling term

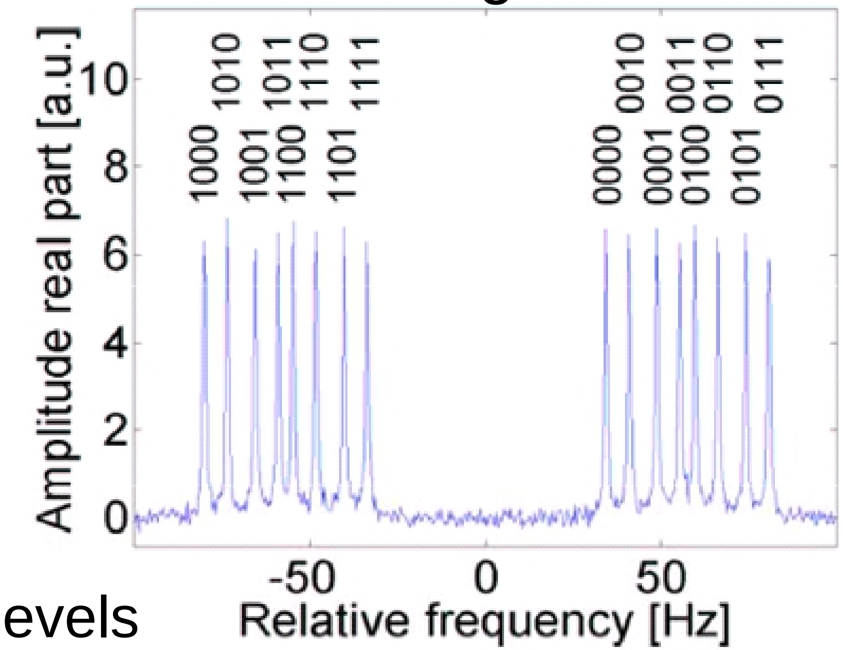
$$\mathcal{H}_J = \hbar \sum_{i<j}^{n} 2\pi J_{ij} I_z^i I_z^j$$

Typical values: *J* up to few 100 Hz

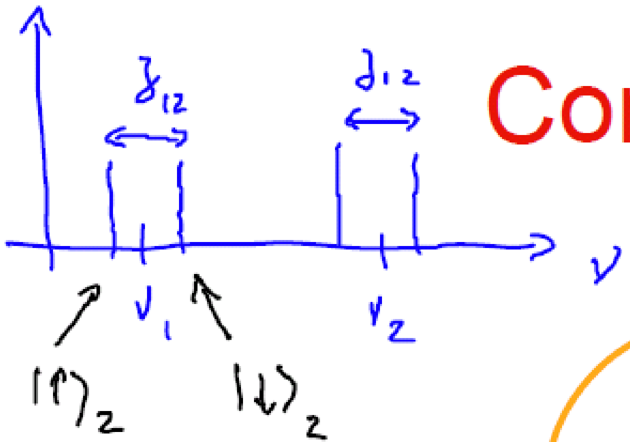


16 configurations



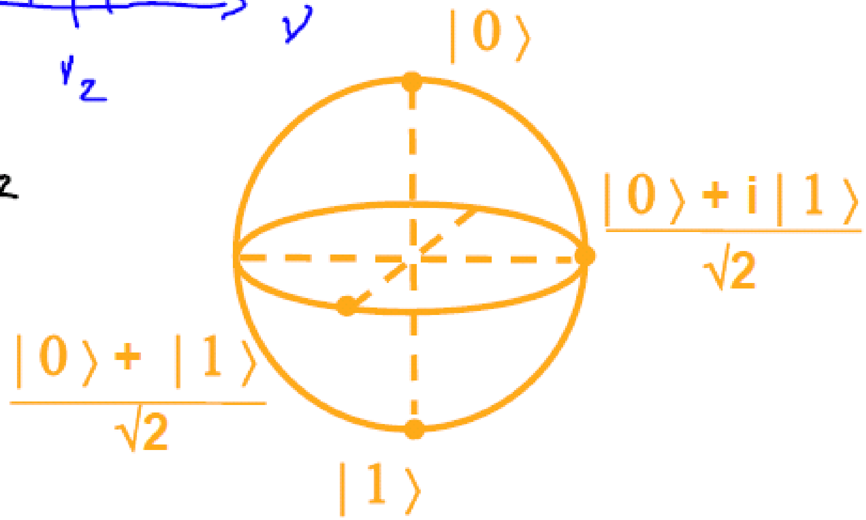


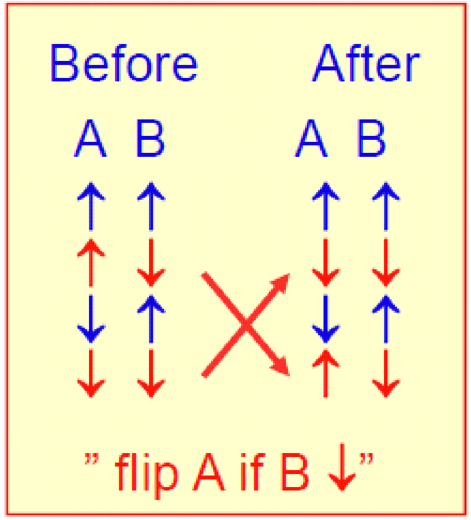
solid (dashed) lines are (un)coupled levels

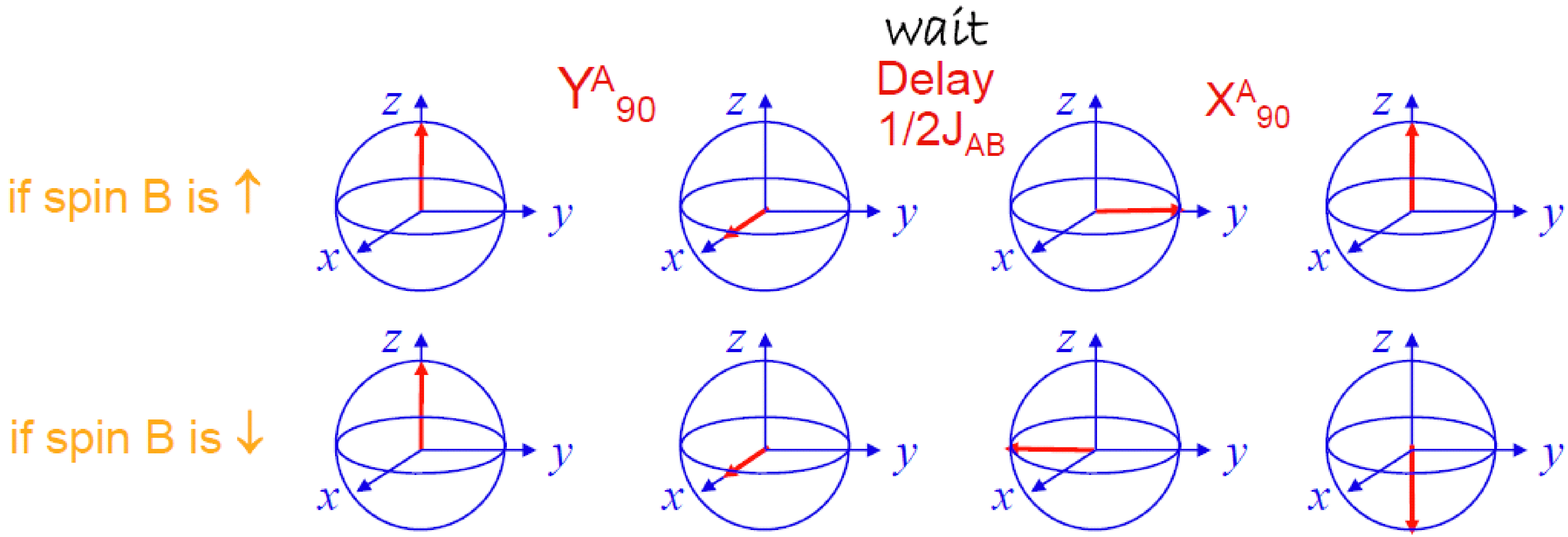


Controlled-NOT in NMR

A target bit
B control bit



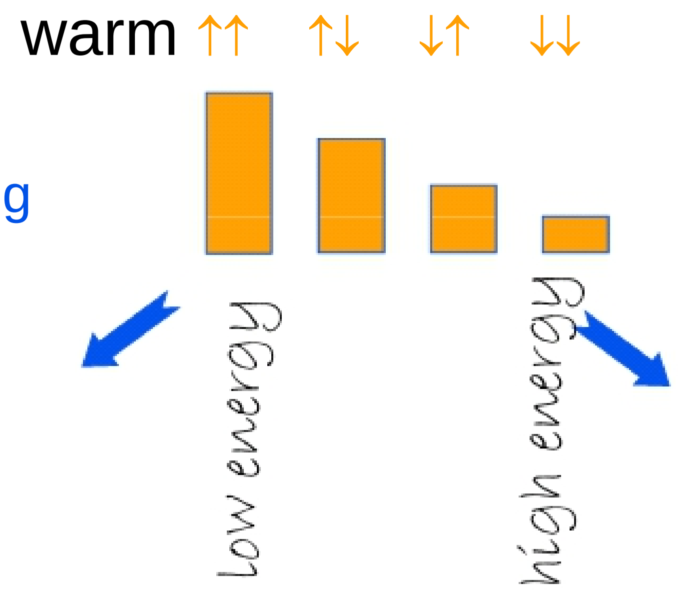


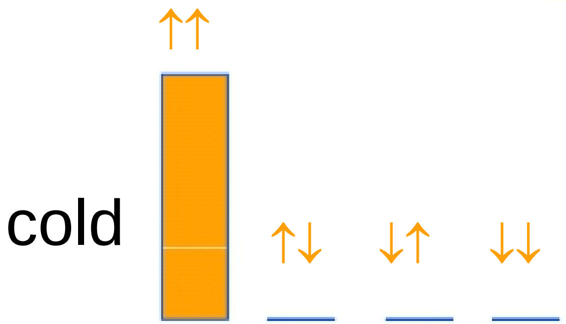


different rotation direction depending on control bit → time

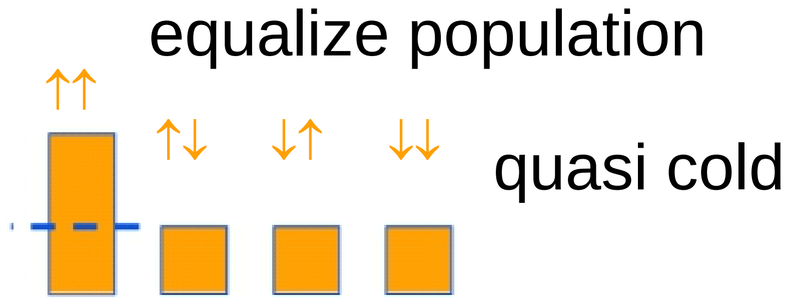
Making room temperature spins look cold

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

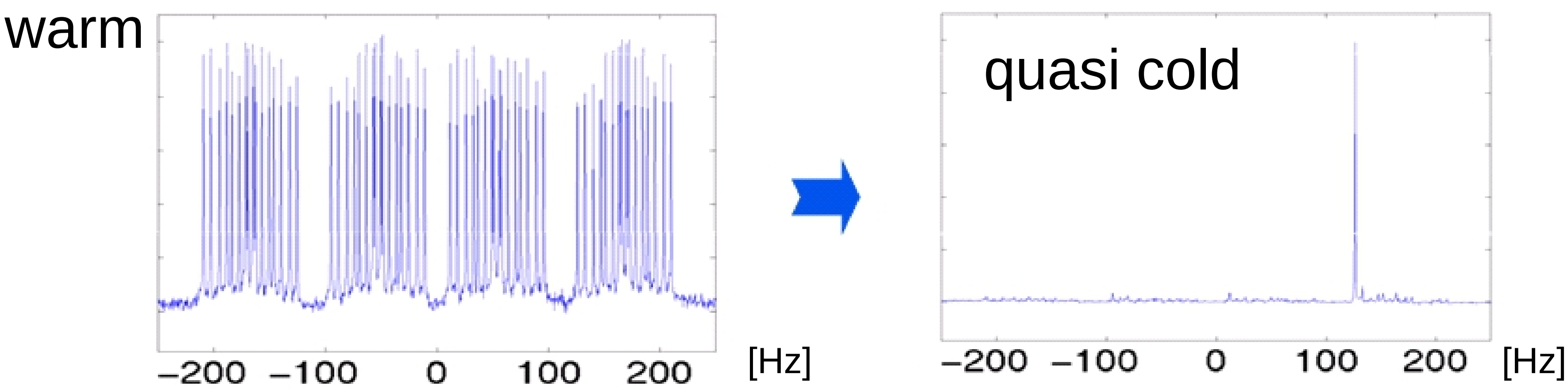




Effective pure state
(Gershenfeld&Chuang, Science '97, Cory, Havel & Fahmi, PNAS '97)

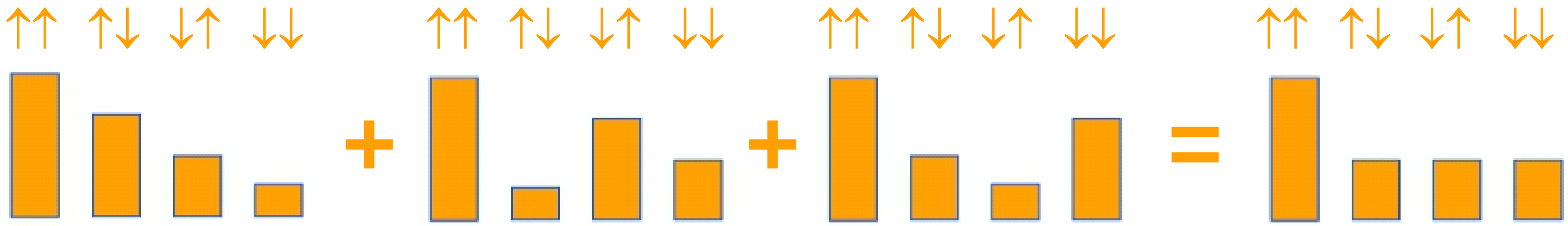


Look exactly like cold spins !



Effective pure state preparation

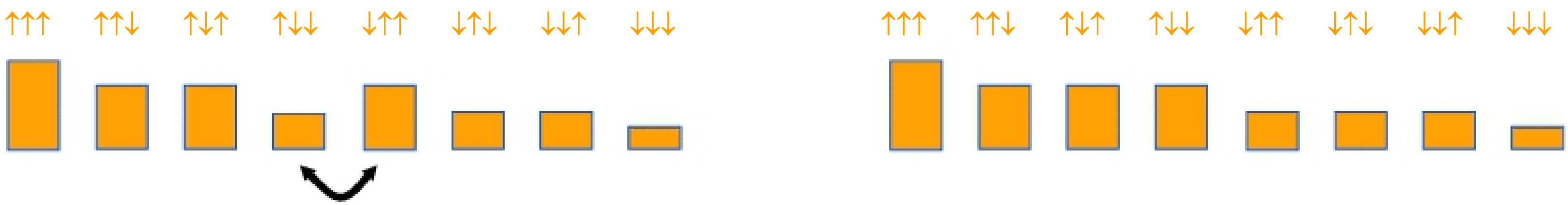
(1) Add up 2^N-1 experiments (Knill,Chuang,Laflamme, PRA 1998)



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

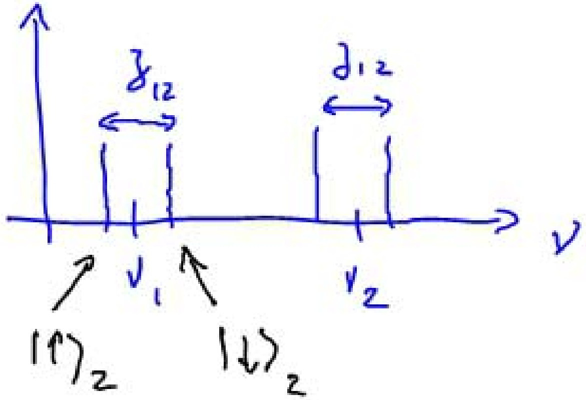
prepare equal population (on average) and look at deviations from equilibrium.

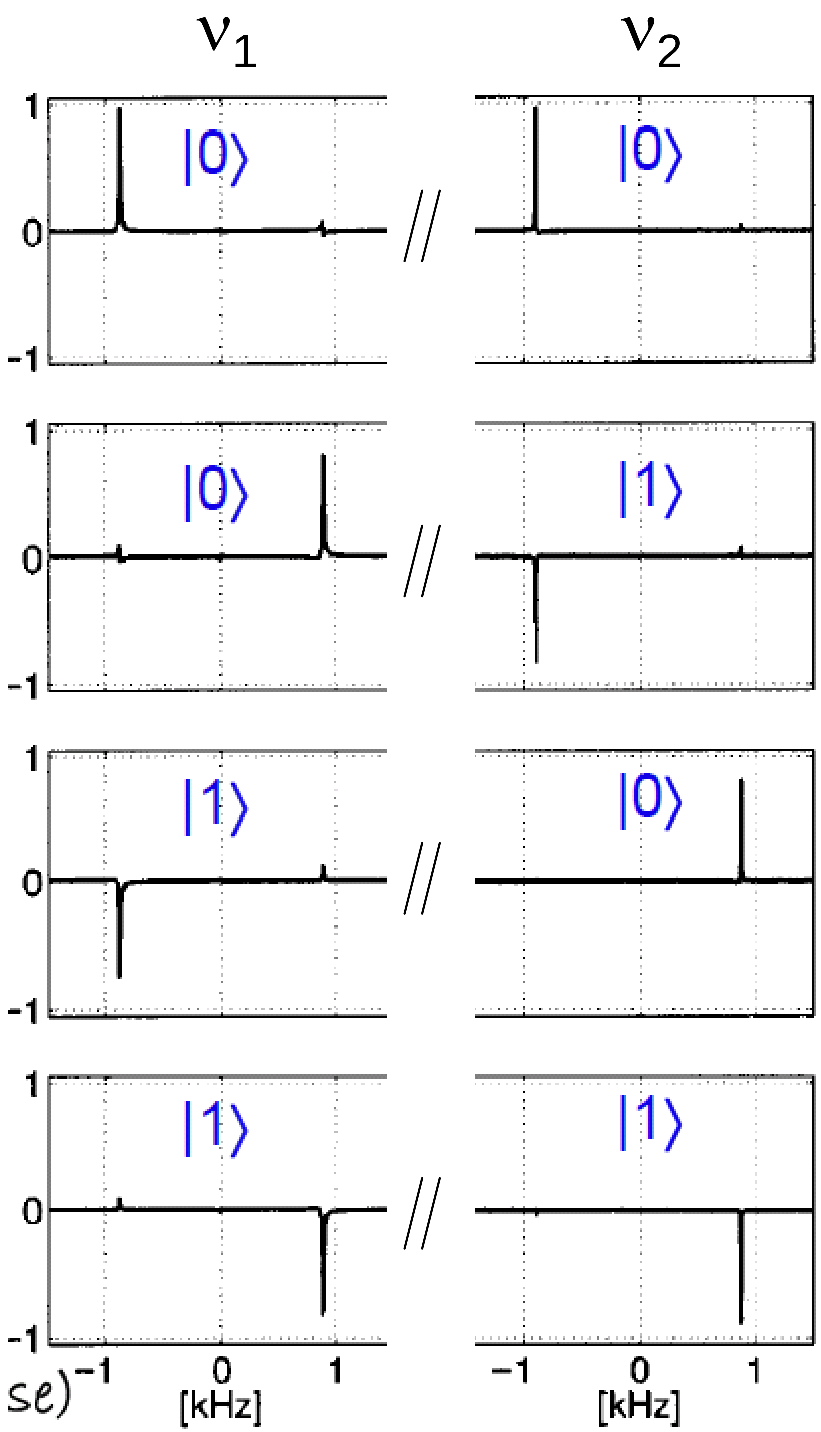
(2) Work in subspace (Gershenfeld&Chuang, Science 1997)



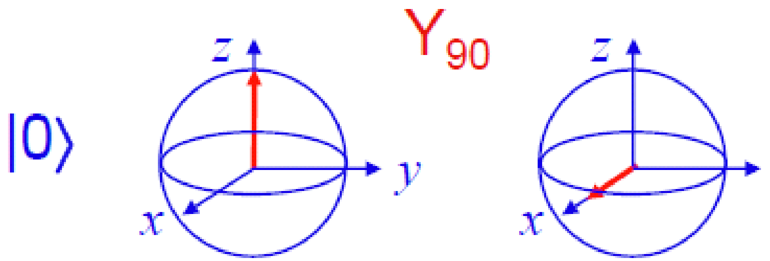
compute with qubit states that have the same energy and thus the same population.

Read-out in NMR

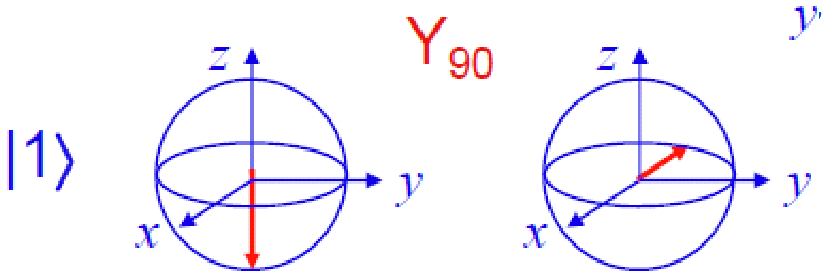




Phase sensitive detection



positive signal for |0>



negative signal for |1>

NMR Spectrometer

Computer – Console – Superconducting magnet

Transmission / Receiver coil

Liquid-state NMR

Survey of NMR quantum computing

Principles of NMR QC

⇨ Molecule Selection

Summary: Pros & Cons

Molecule selection

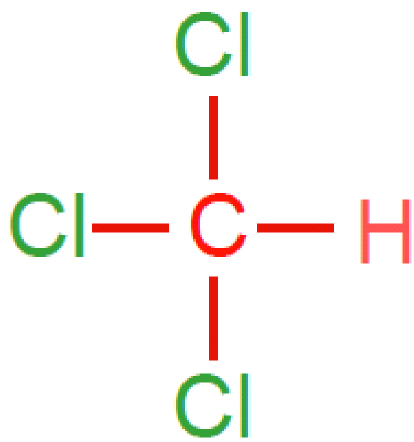
A quantum computer is a *known* molecule.
Its desired properties are:

- spins 1/2 (^{1}H, ^{13}C, ^{19}F, ^{15}N, ...)
- long T_1's and T_2's
- heteronuclear, or large chemical shifts → required to make spins of same type addressable
- good J-coupling network (clock-speed)
- stable, available, soluble, ...

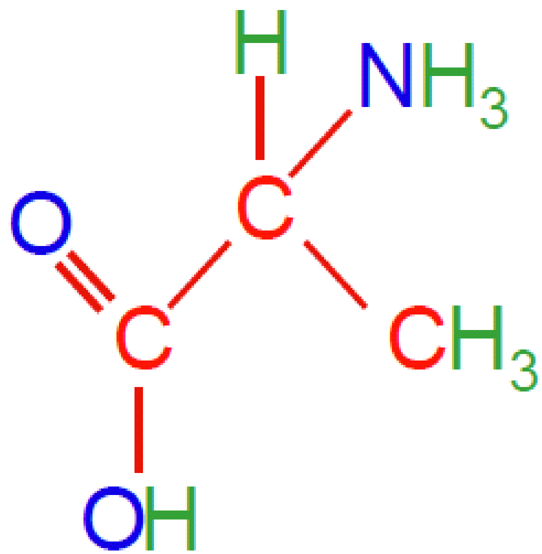
Quantum computer molecules (1)

red nuclei are used as qubits:

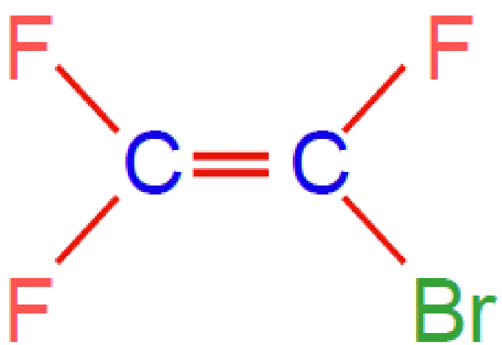
Grover / Deutsch-Jozsa



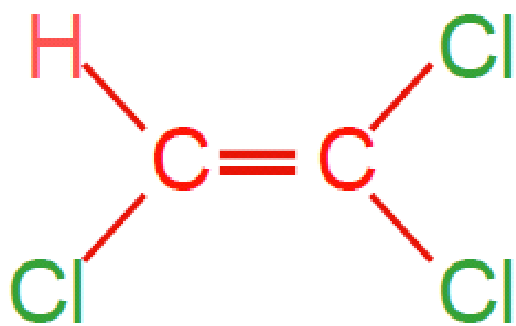
Q. Error correction



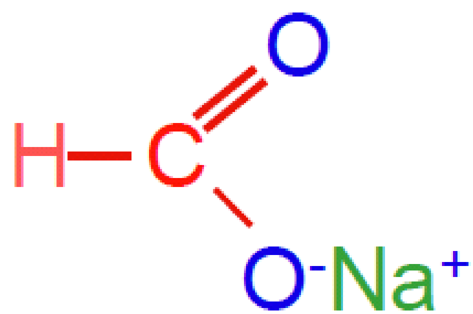
Logical labeling / Grover



Teleportation

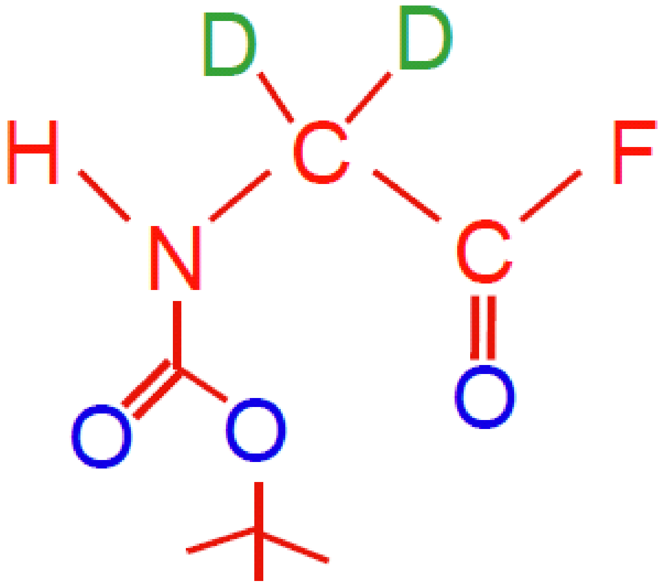


Q. Error Detection

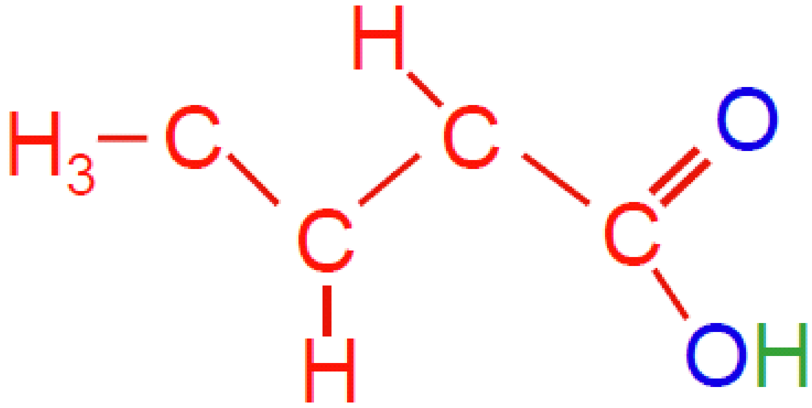


Quantum computer molecules (2)

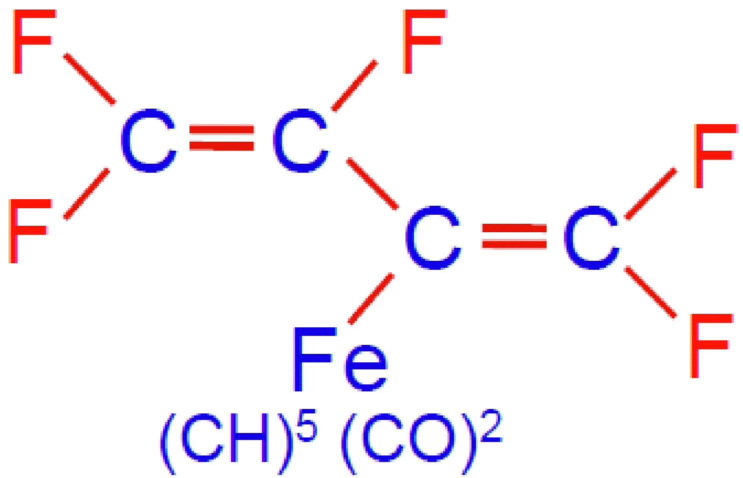
Deutsch-Jozsa



7-spin coherence



Order-finding



Liquid-state NMR

Survey of NMR quantum computing

Principles of NMR QC

Molecule Selection

➡ 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

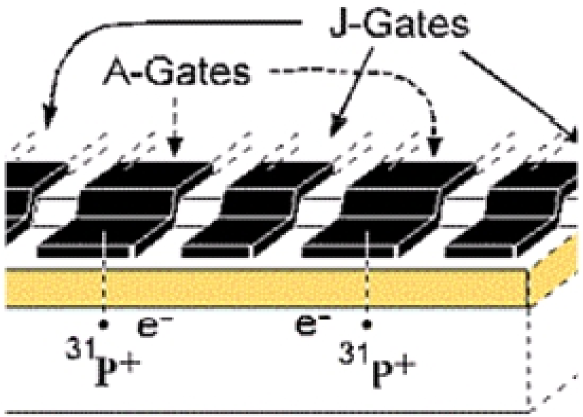
Later (homonuclear molecules)

*J c*oupling during RF pulses

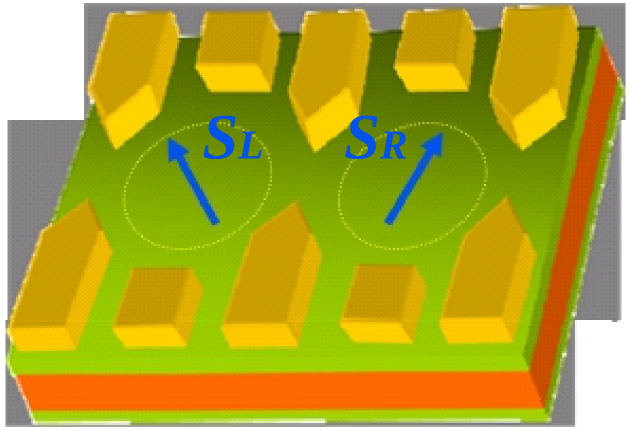
Finally

decoherence

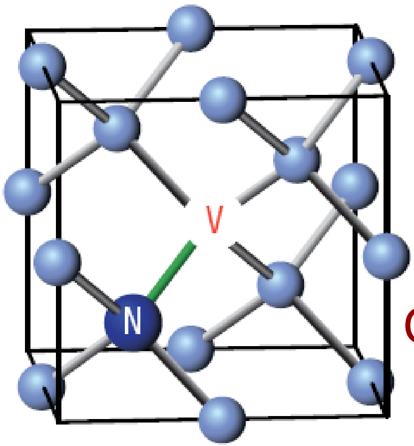
Electron spin qubits



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

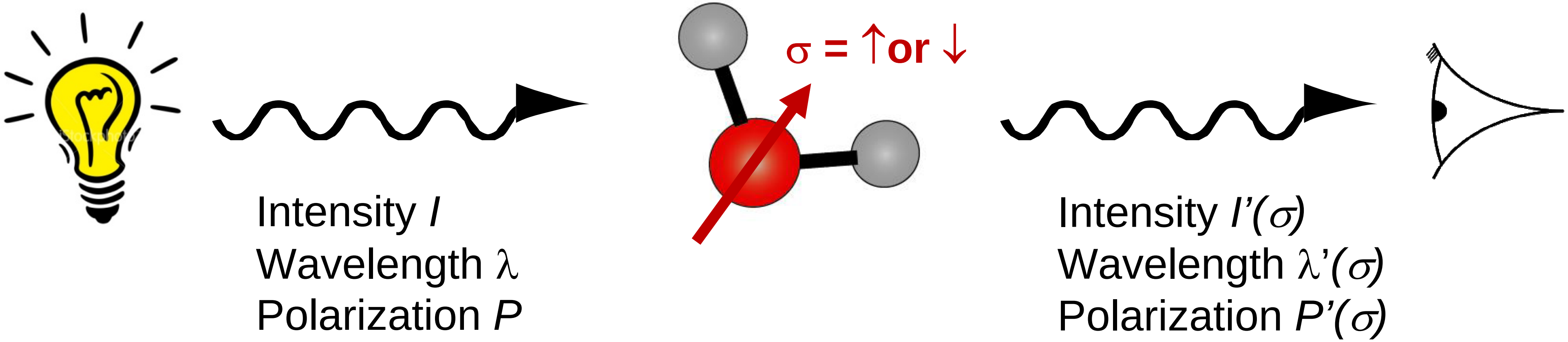
Environment: Diamond host material

Applications

Optically-detected magnetic resonance (ODMR)

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

<u>Requirement:</u> Optical photon must be correlated with spin state



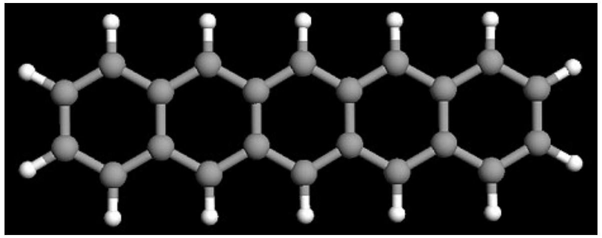
Optically detected magnetic resonance

Some History

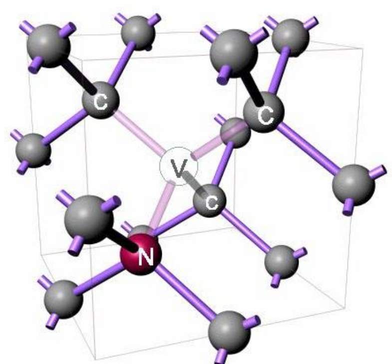
- Optical detection of paramagnetism in phenantren (Kwiram, 1967)

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

- Optical detection of magnetic resonance in a single pentacene molecule
  Wrachrup, Moerner (1993)

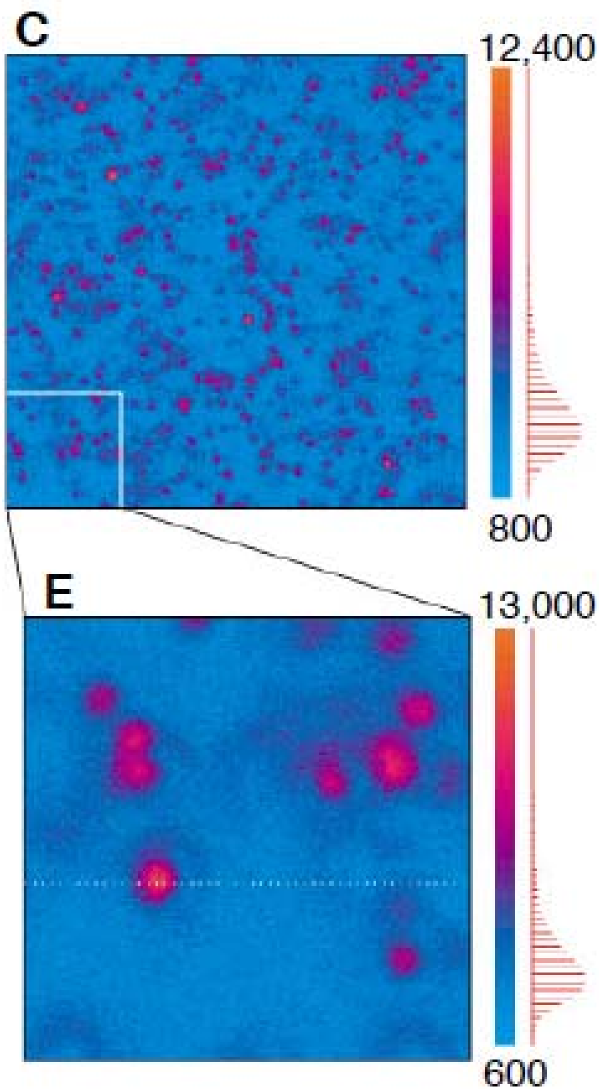


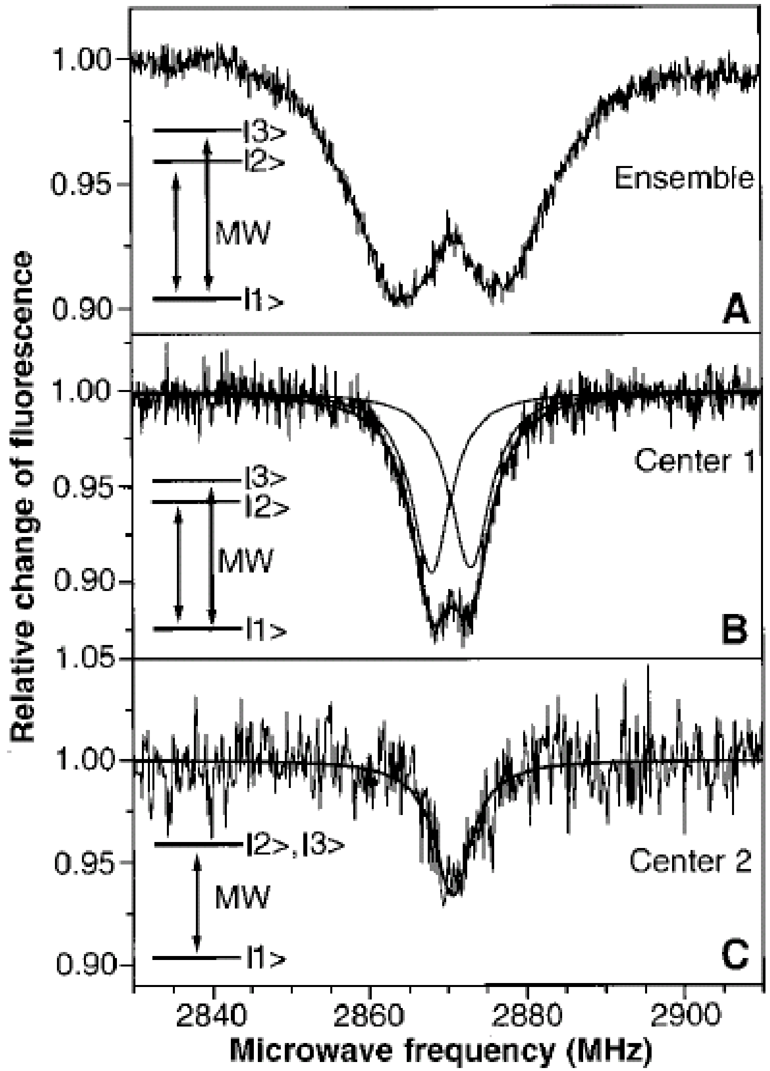
- Optical detection of single nitrogen vacancy centers in diamond:
  Gruber, Wrachtrup (1997)



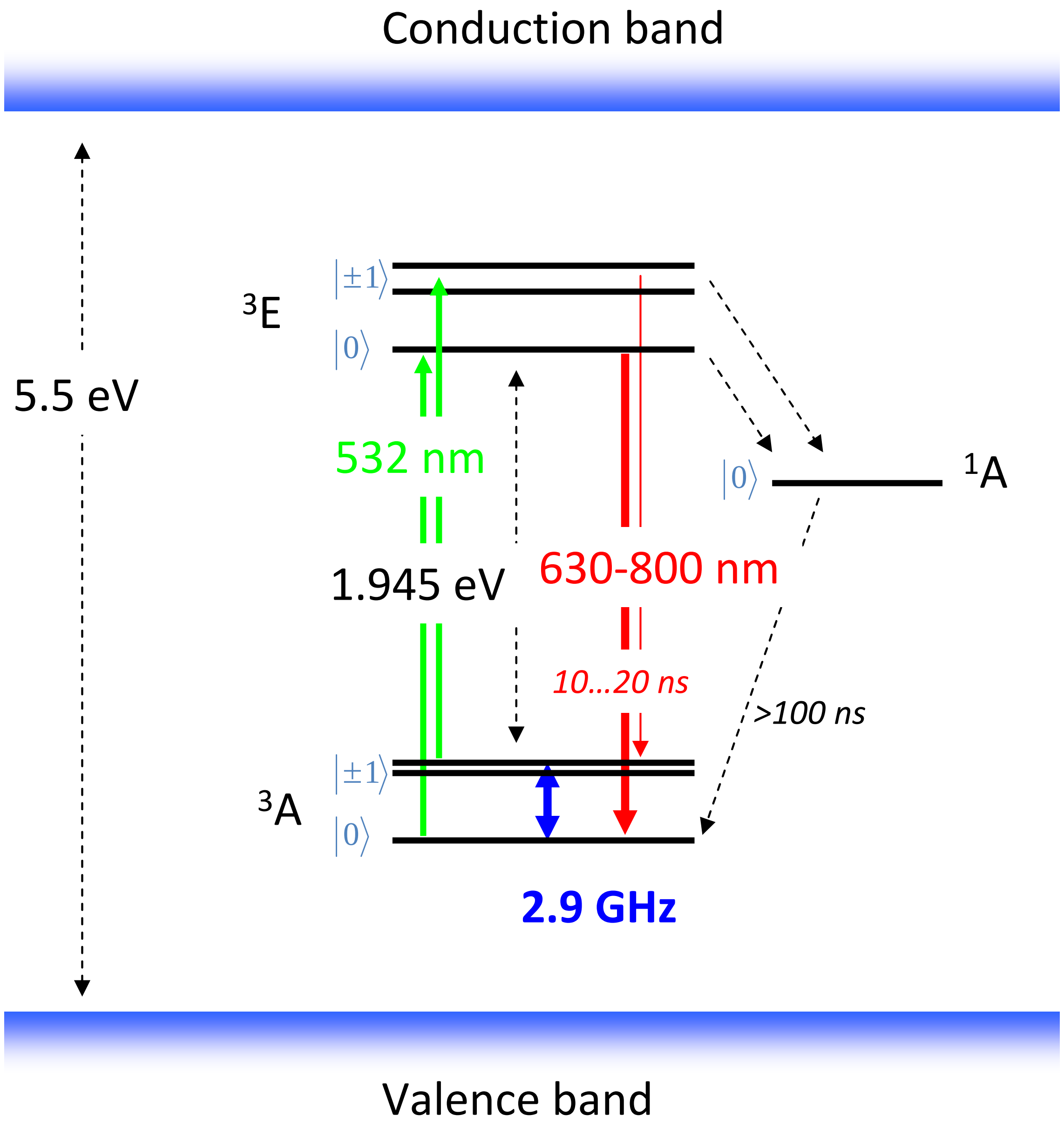
Single spin detection of NV centers

Gruber, Science 1997





Readout and Polarization of the NV center



Readout:

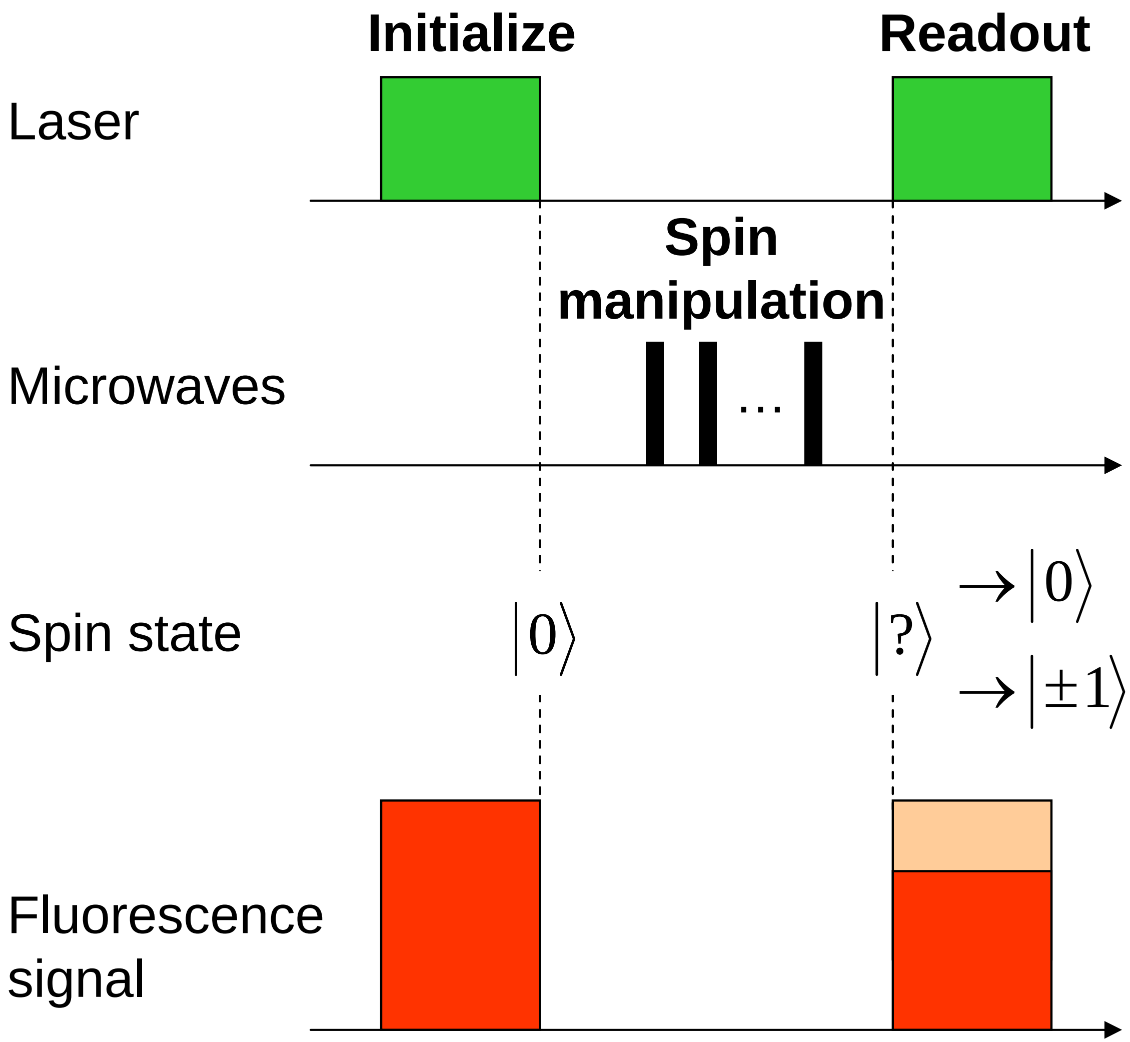
•m_s = 0 scatters 30% more light than m_s = ±1

•Many readout cycles needed to detect spin state

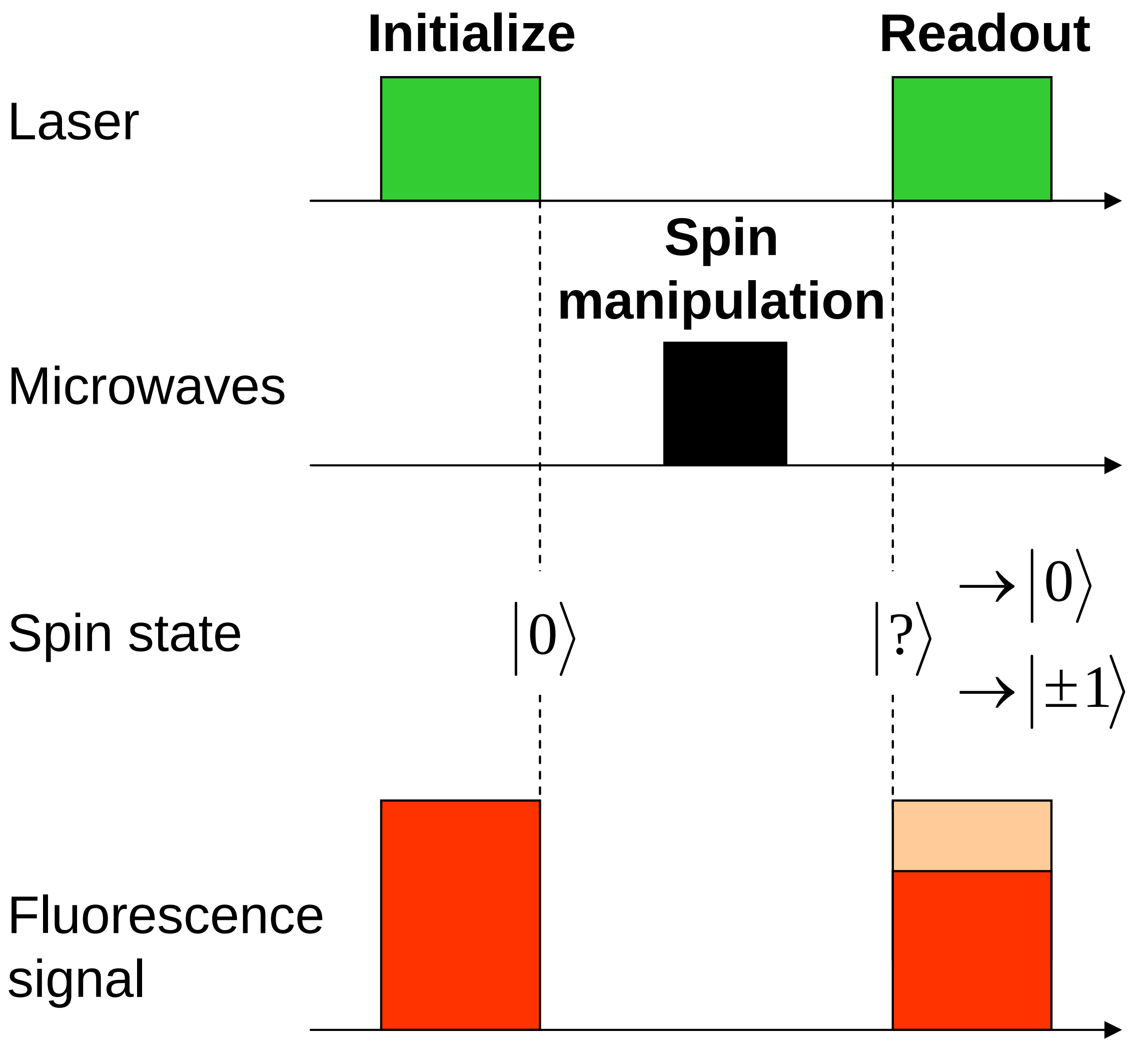
Polarization ("Reset"):

•Illumination pumps spin into m_s = 0 state (>90% fidelity)

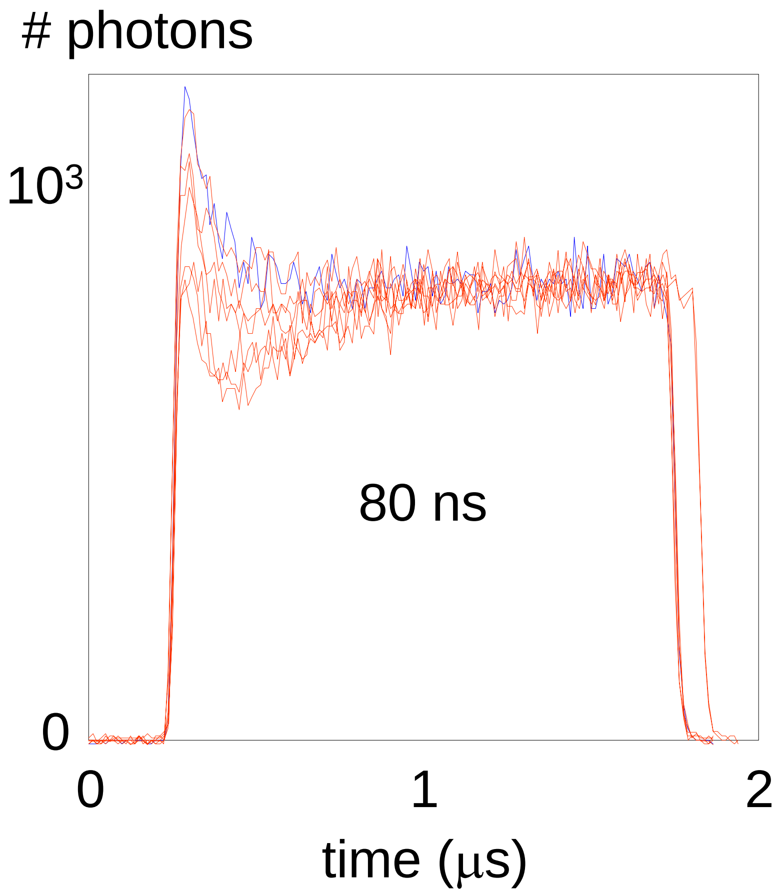
Time-Resolved Experiments



Time-Resolved Experiments



- Rabi oscillations



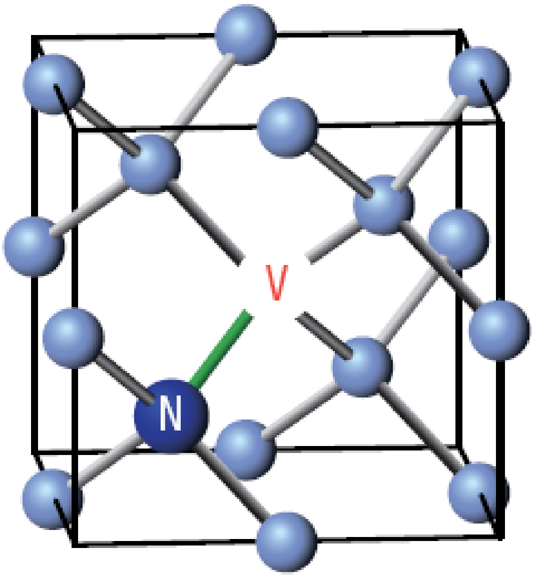
Spin Hamiltonian

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

Zero field splitting
(2.87 GHz)

Electron Zeeman
(2.8 MHz/Gauss)

Hyperfine coupling to ^{14}N
(~2.2 MHz)

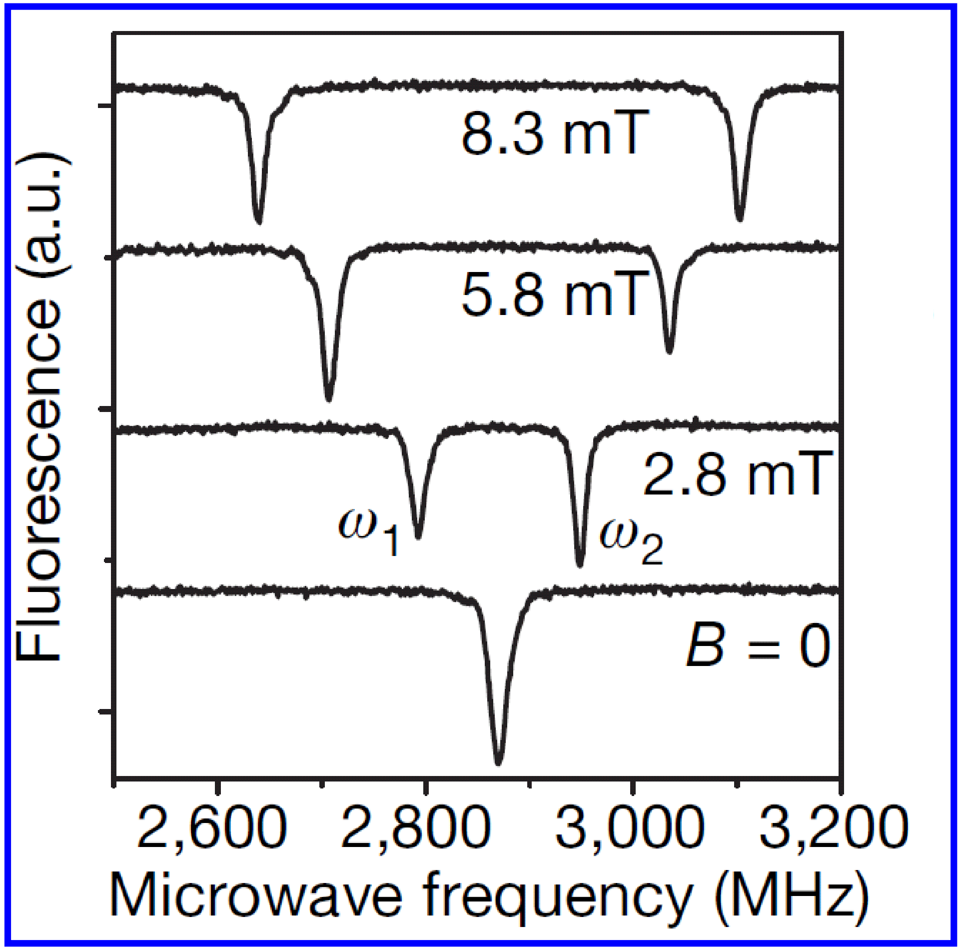


Jelezko, Journal of Phys. Cond Mat. 2006

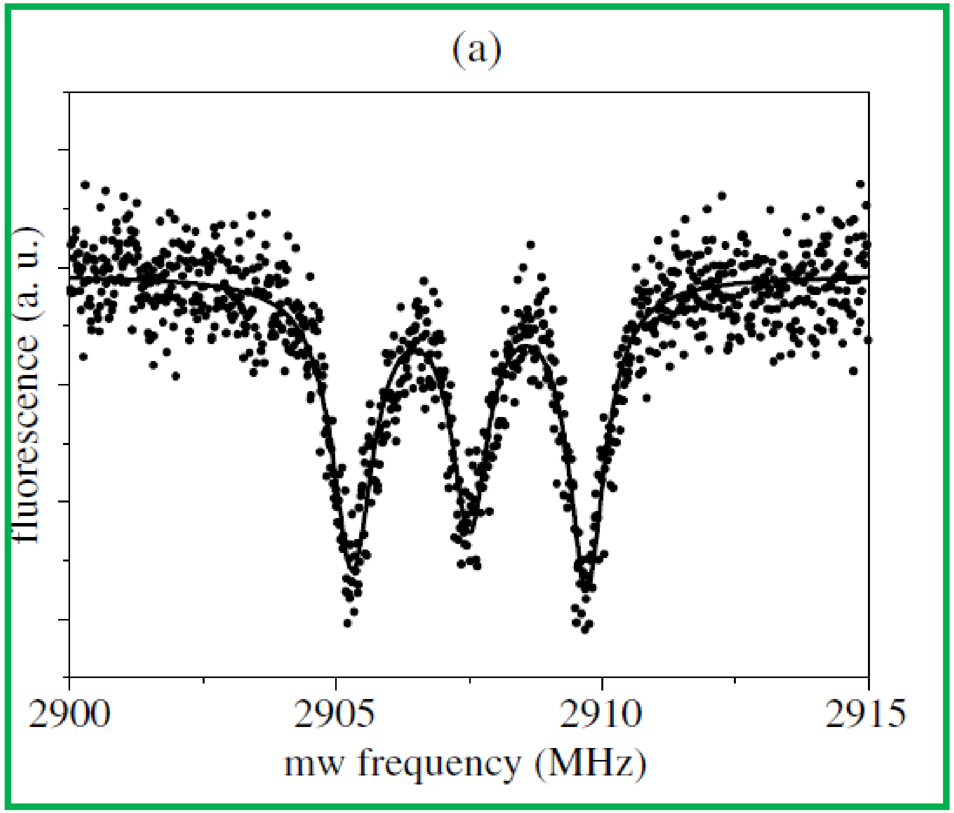
Spin Hamiltonian

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

Zeeman



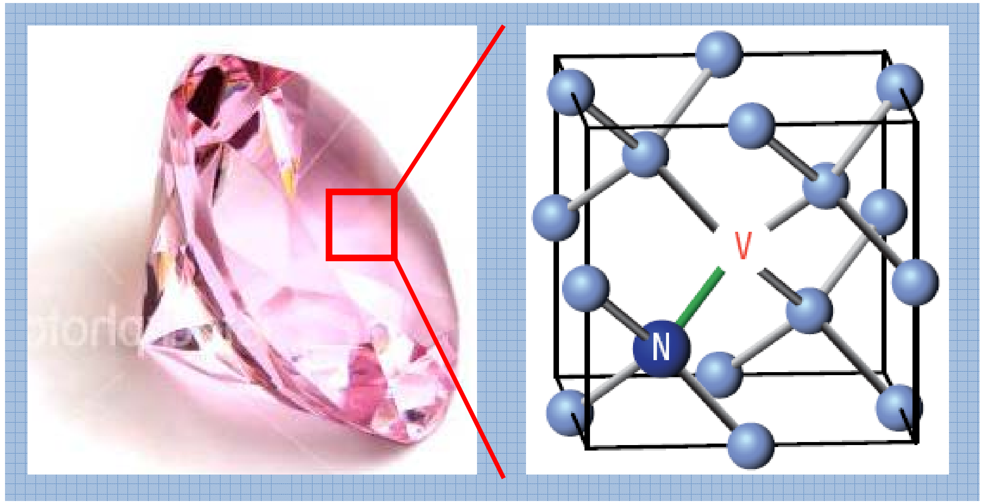
Hyperfine



NV centers in diamond

Some properties:

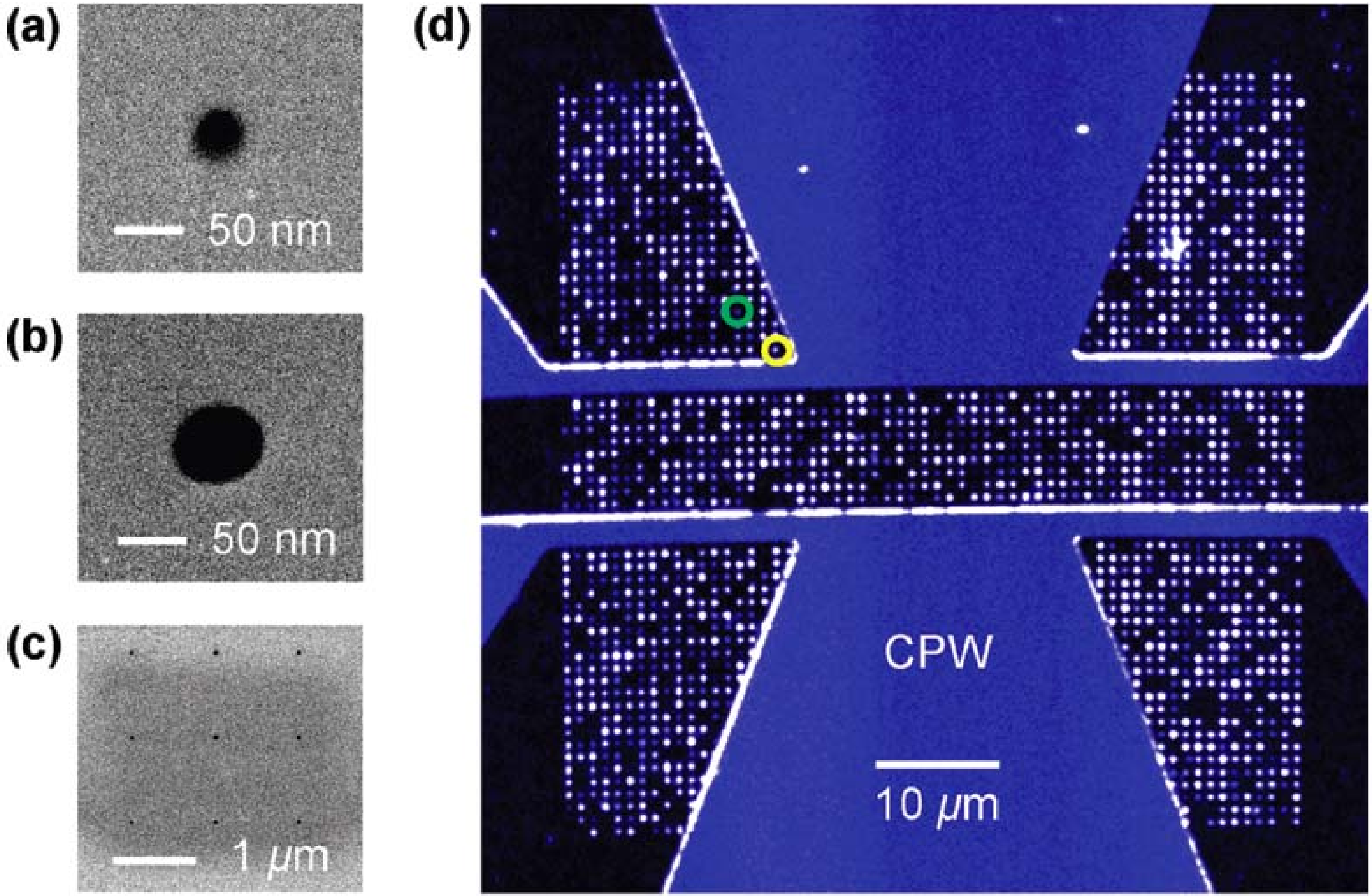
- Single photon emitter
- Optically stable:
  No bleaching, no blinking
- High quantum yield ~70%
- Room temperature
- Long spin coherence times >1ms
- In nanodiamonds down to 5 nm
- Excellent chemical stability
- Non-toxic biomarkers
- Inexpensive!
- …



Nitrogen Vacancy defect in diamond

Fabrication – Ion implantation

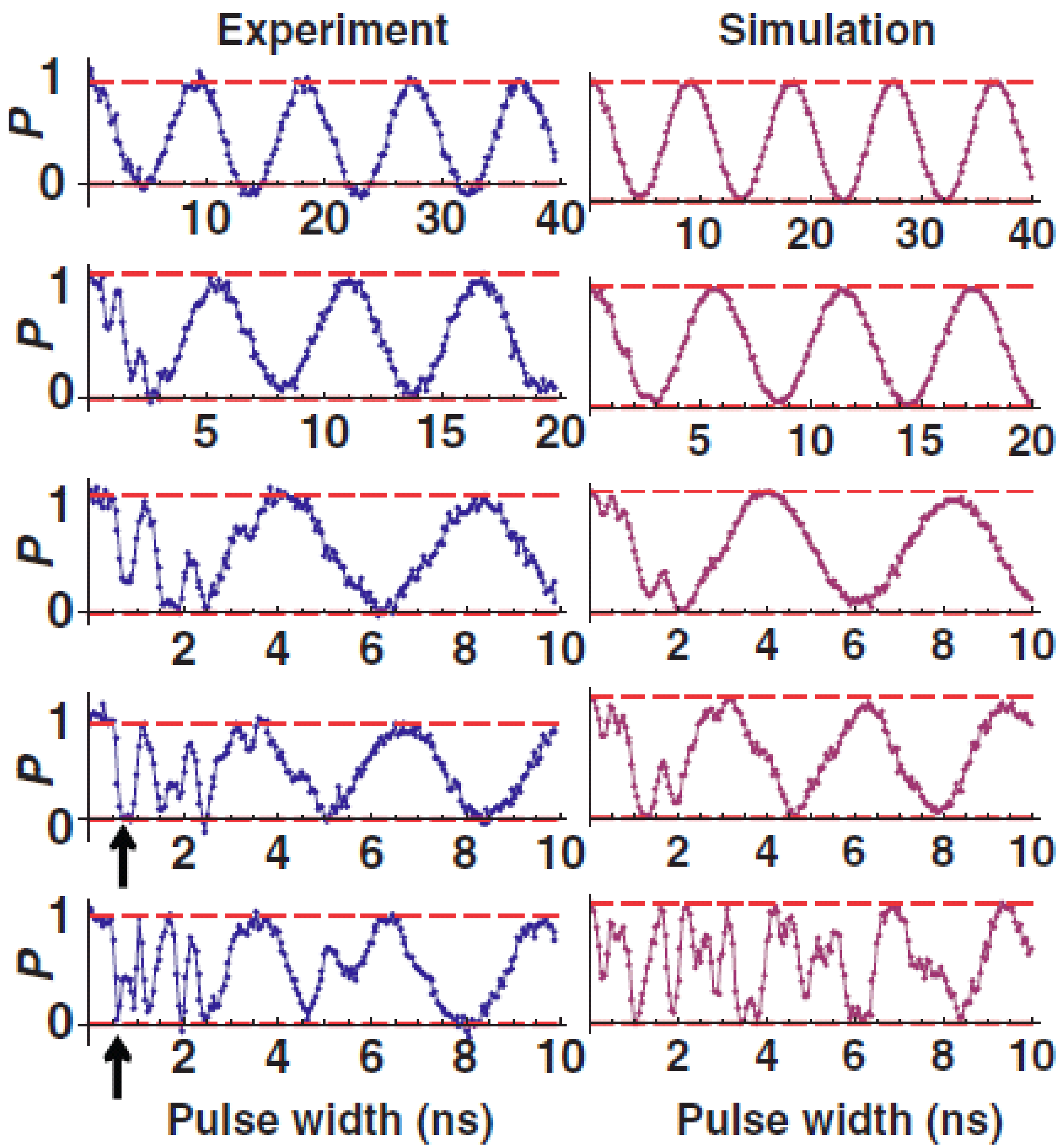
NV centers implanted into single crystal diamond, then patterned with waveguide

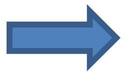


Toyli, Nano Letters, 2010

Rapid spin manipulation by waveguides

Rabi Oscillations





Spin inversion within ~ 1 ns

Fuchs, Science, 2009

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

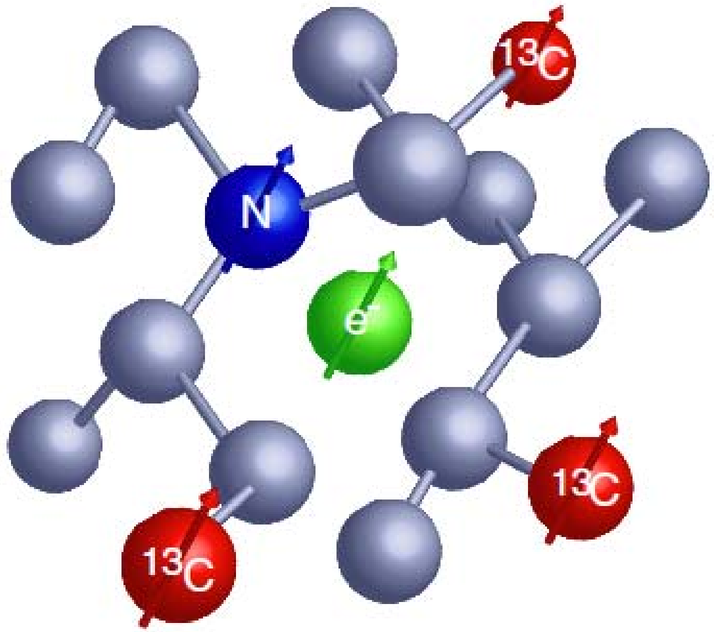
Spin environment

Nuclear spins

- ^{14}**N**V 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)

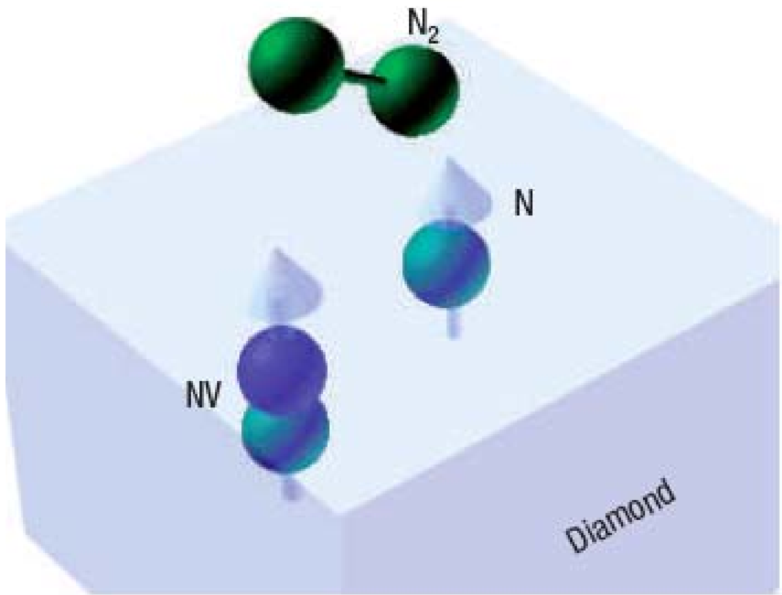
Electron spins

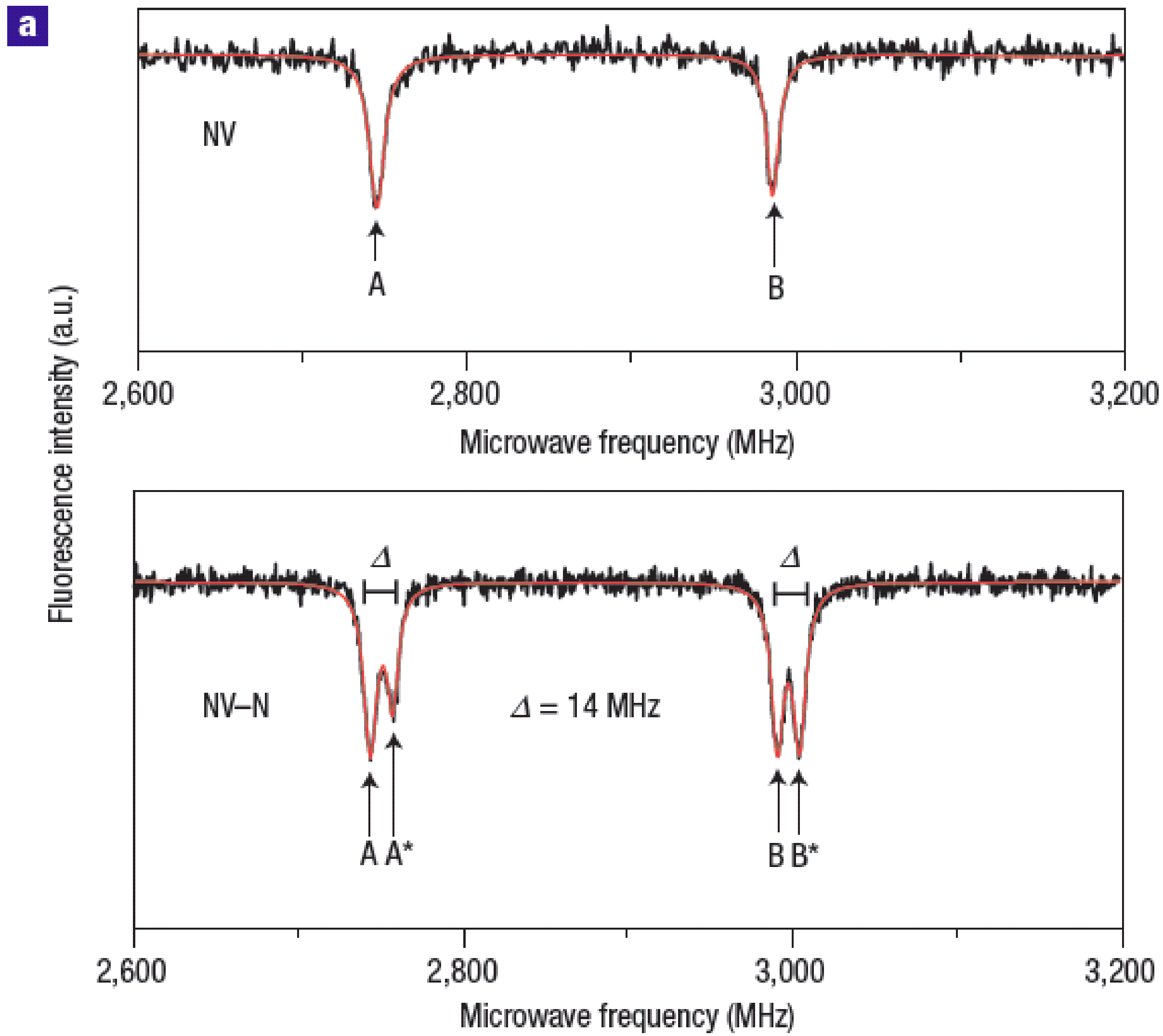
- Nearby **N defect** electron spins (S=1/2) ("P_1 or C centers")
- Nearby other **NV center** (S=1)
- …
- Surface spins (electronic, nuclear)



Other electronic spins

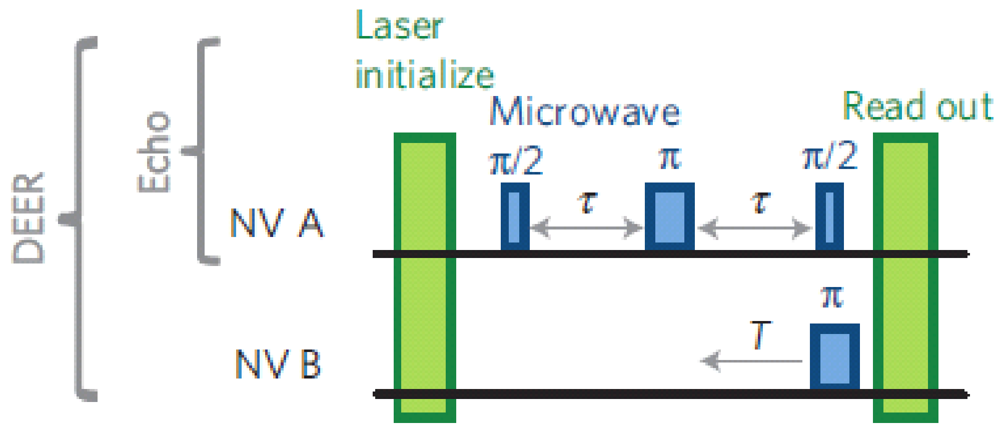
Nearby N defect with S = ½ ("P1 center")

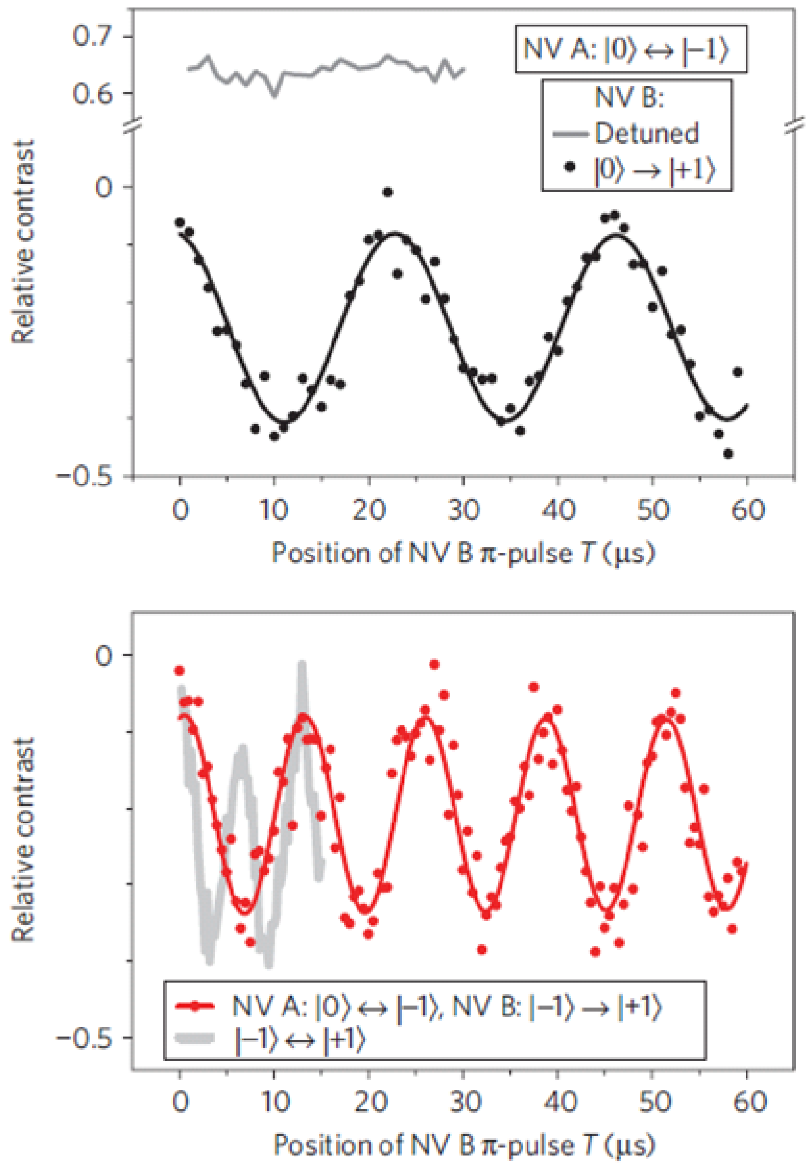


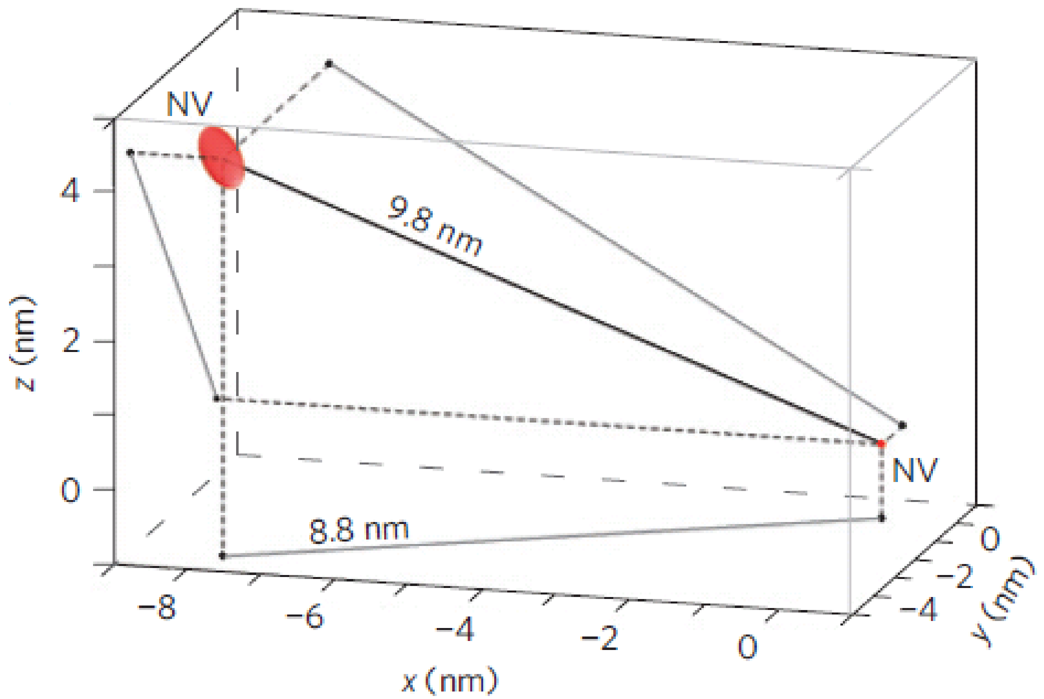


Gaebel, Nature Physics, 2006

Coupling between two NV centers

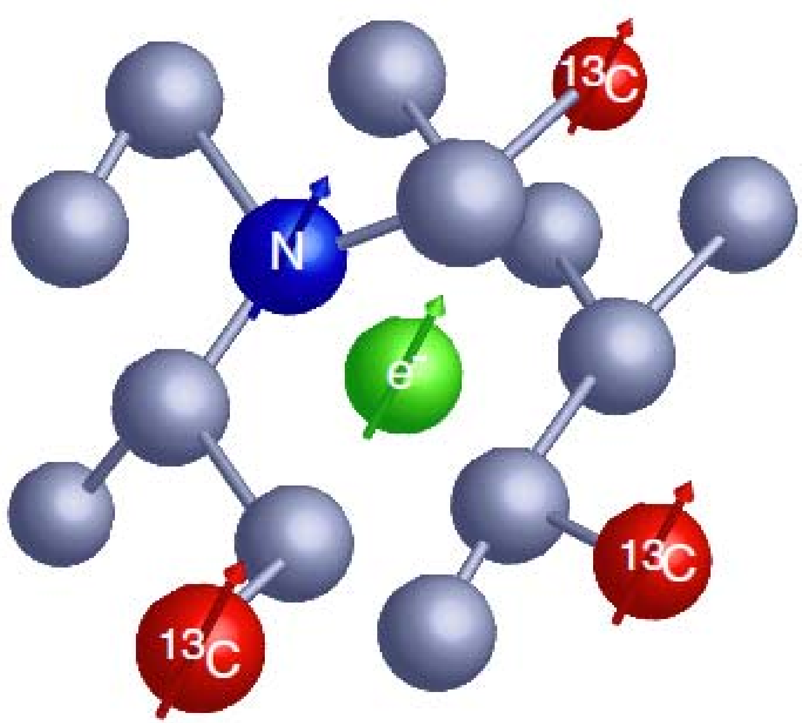






Neumann, Nature Physics, 2010

The ^{13}C nuclear spin environment



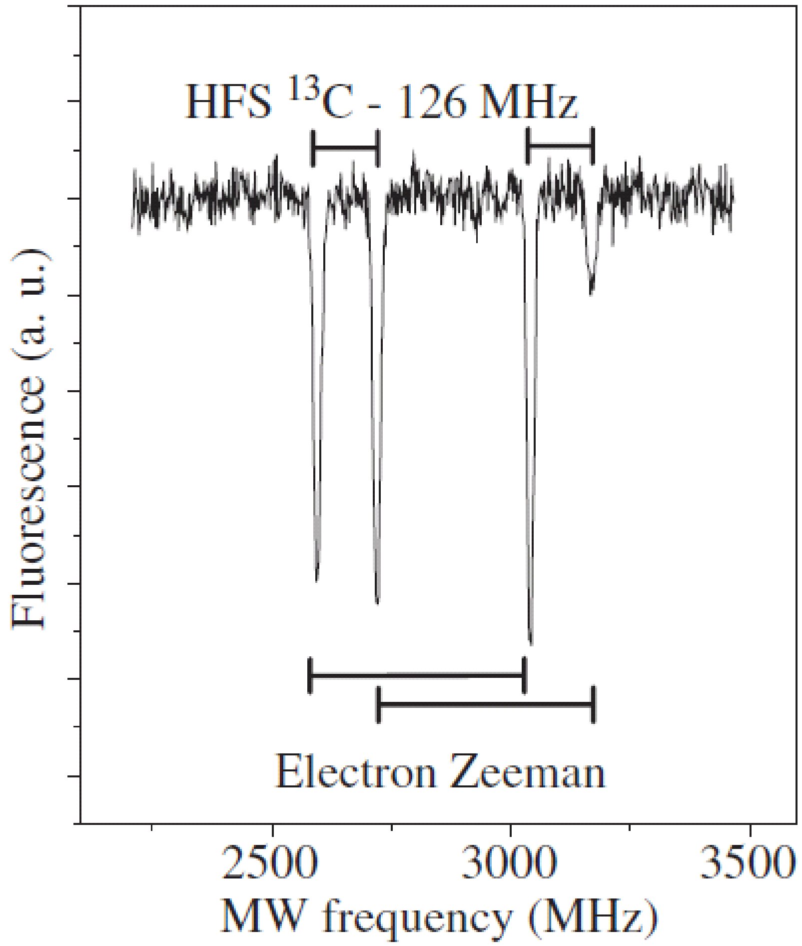
Near ^{13}C spins – resolved lines

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

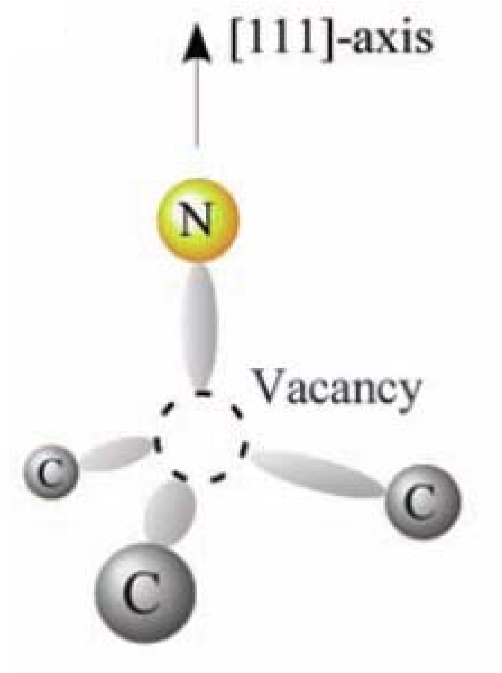
Distant ^{13}C spins – very weak hyperfine coupling (“classical ensemble”)

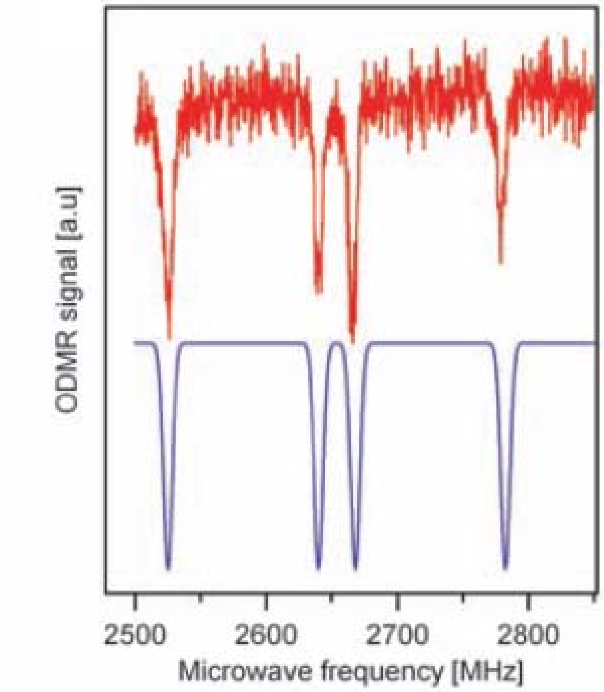
Specific nearby ^{13}C

Two qubits: NV + ^{13}C



Three qubits: NV + ^{13}C + ^{13}C

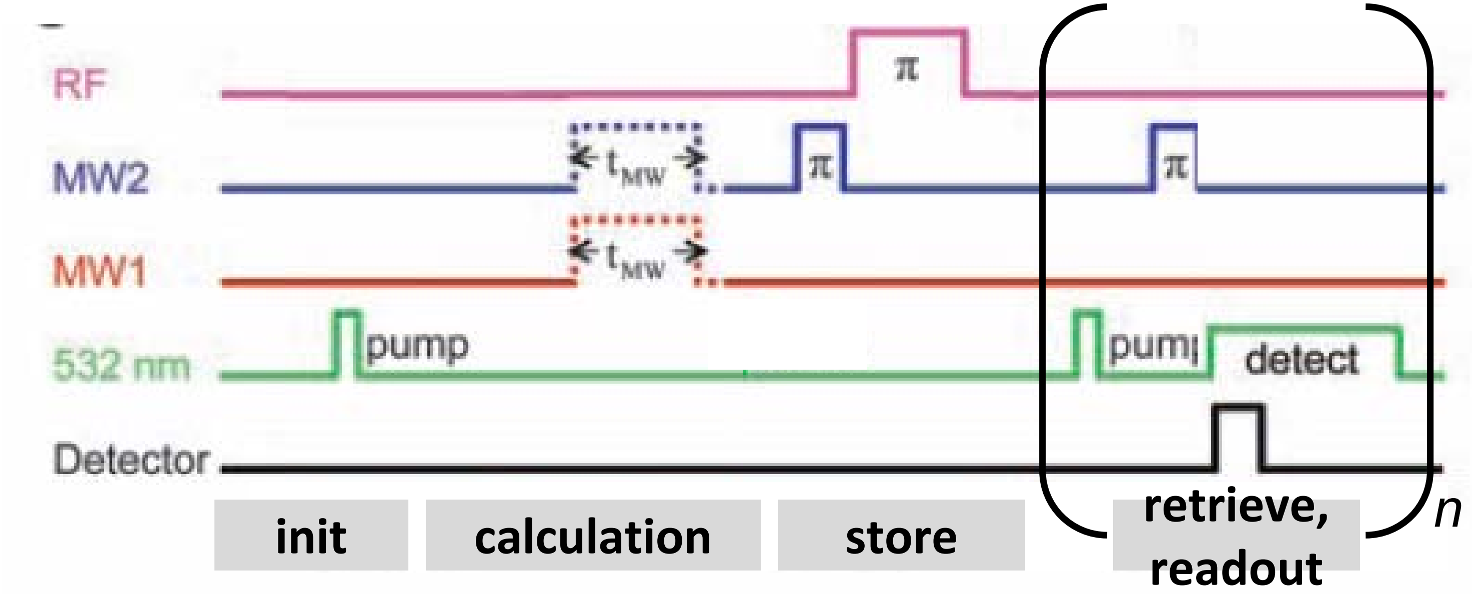


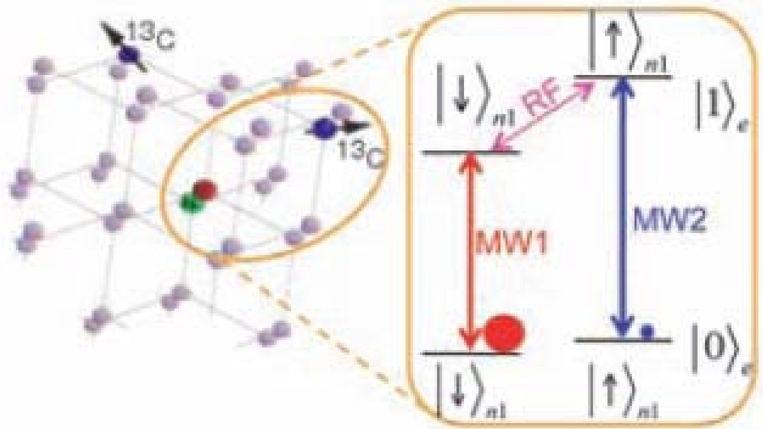


Dutt, Science, 2007

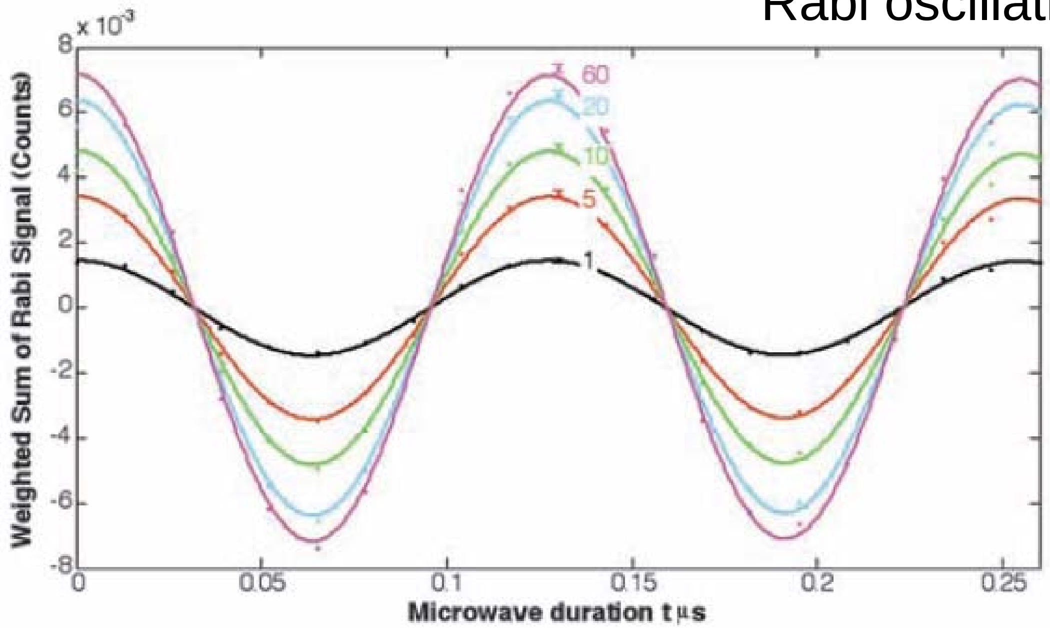
Repetitive readout

Store and Retrieve NV spin state with nearby ^{13}C nucleus





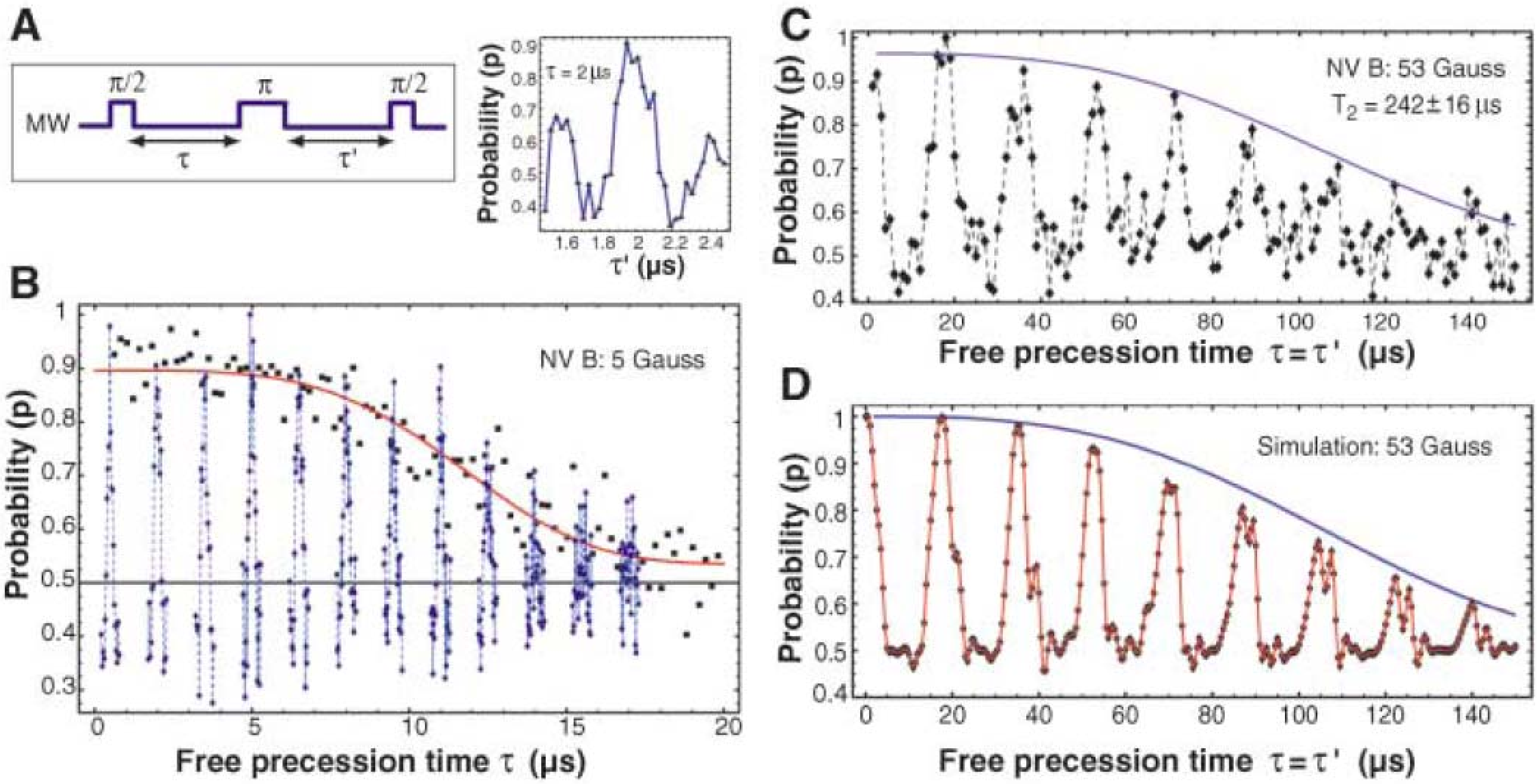
Example:
Rabi oscillation



Jiang, Science, 2009

Distant ^{13}C spin bath

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

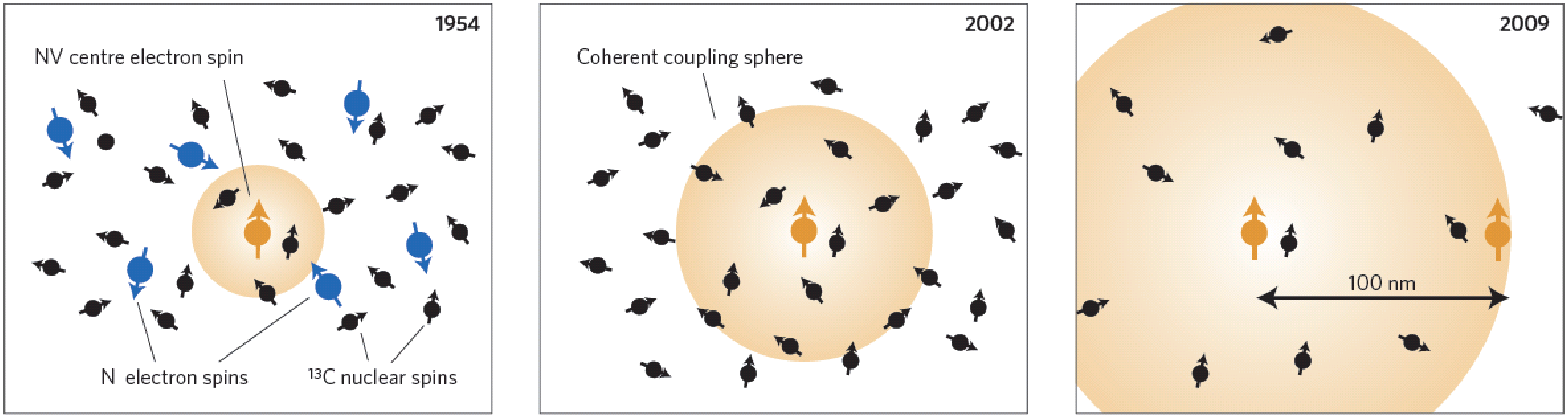


Childress, Science, 2006

Eliminating ^{13}C nuclear spin bath

The materials scientists' way …

^{13}C 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

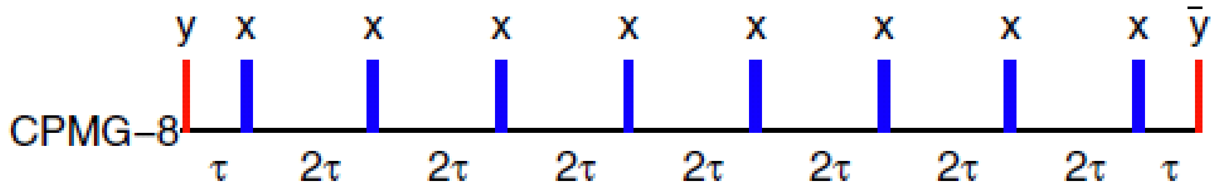


Balasubramanian, Nature Materials, 2009

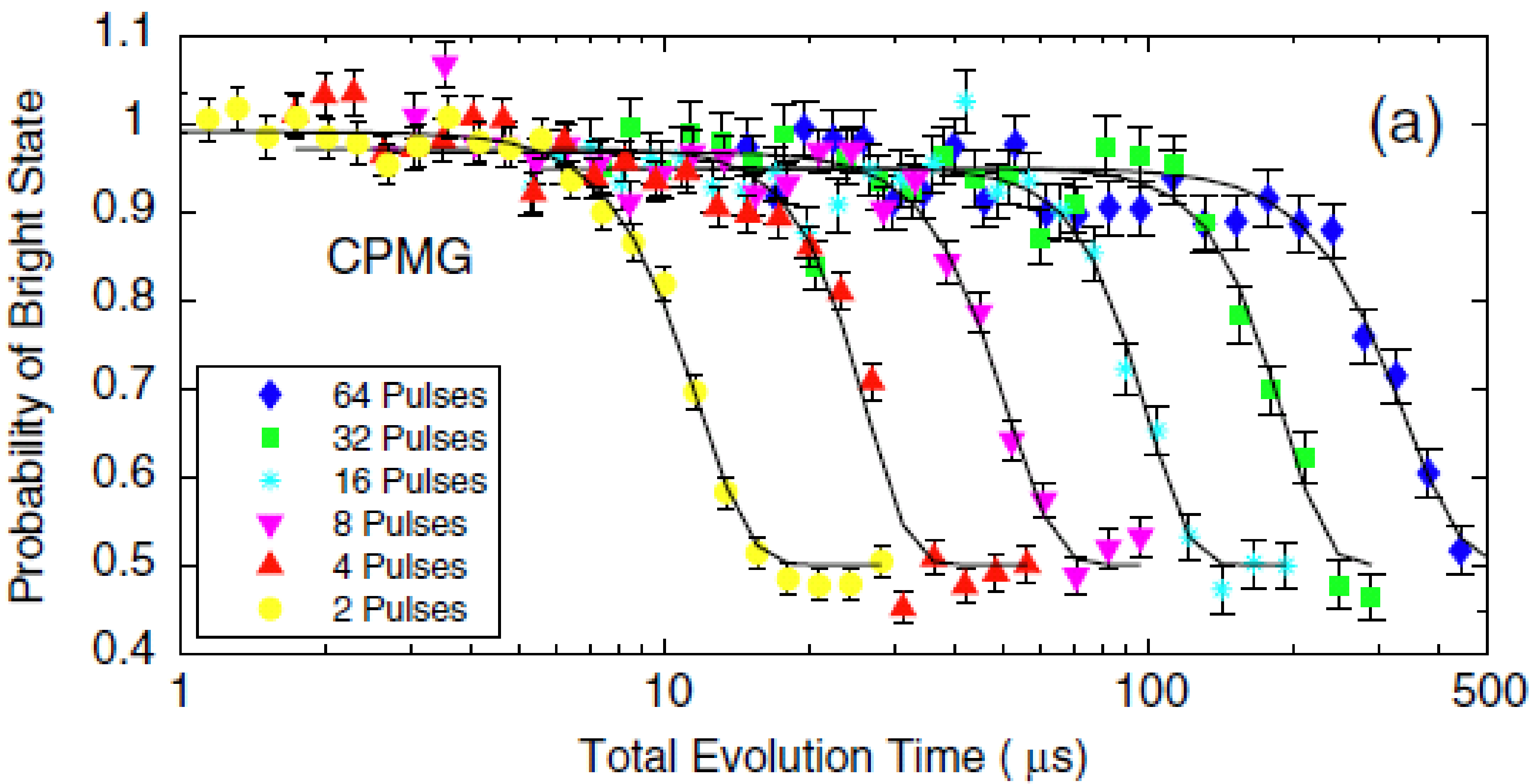
Eliminating ^{13}C nuclear spin bath

… 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

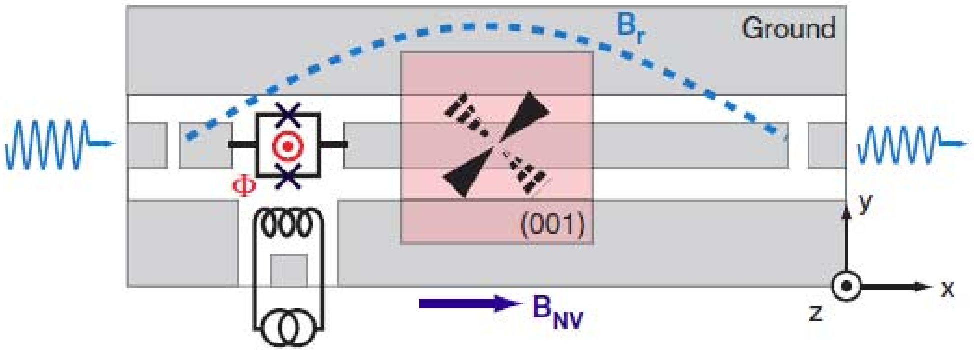
Environment: Diamond host material

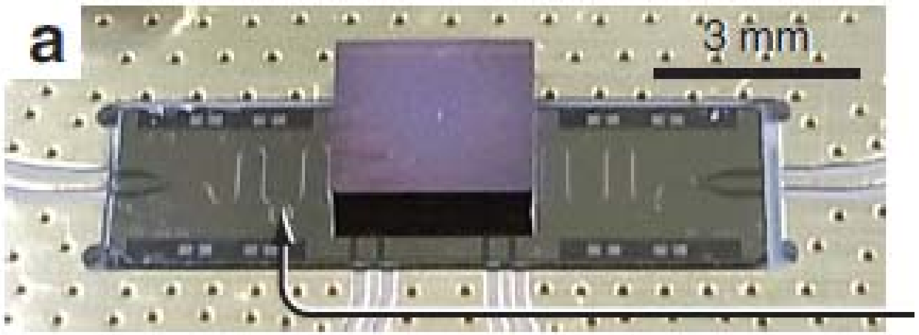
➡ Applications

Hybrid implementations

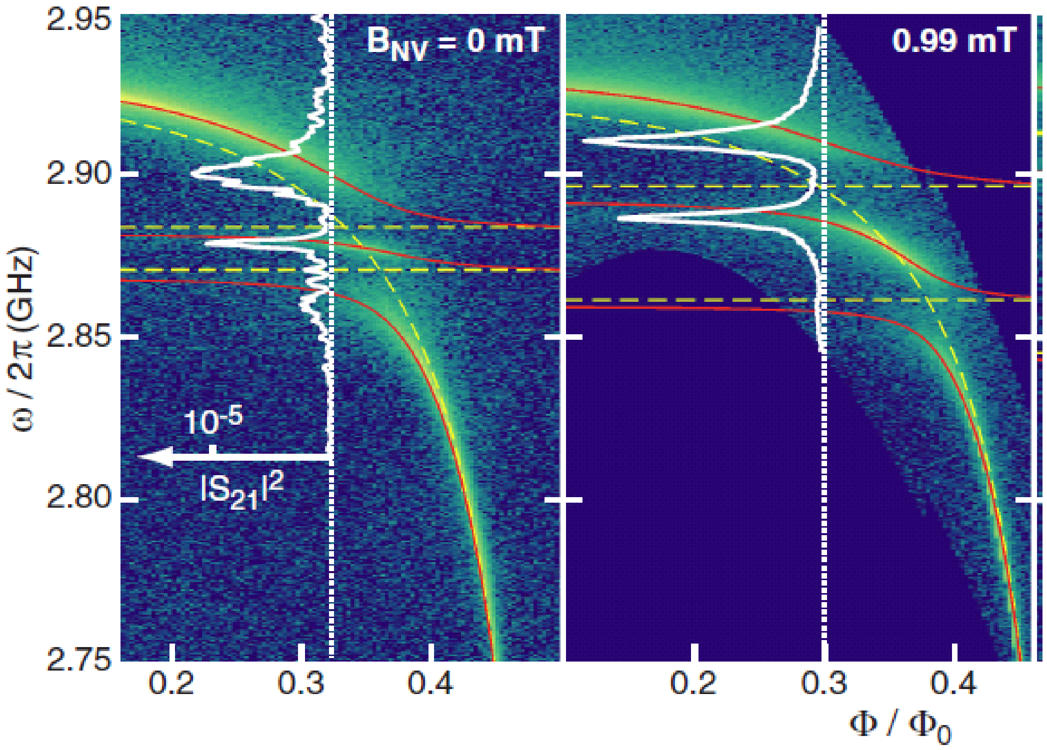
NV centers to superconducting microwave resonator

Arrangement





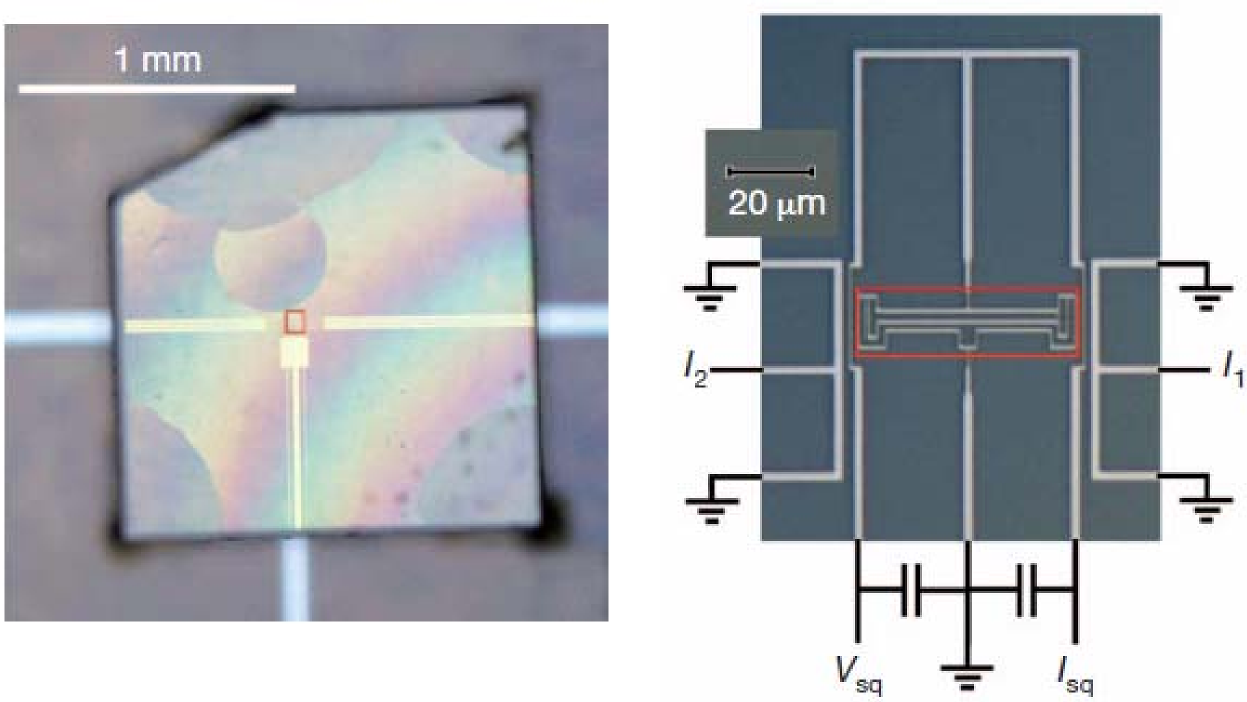
Transmission vs. Frequency



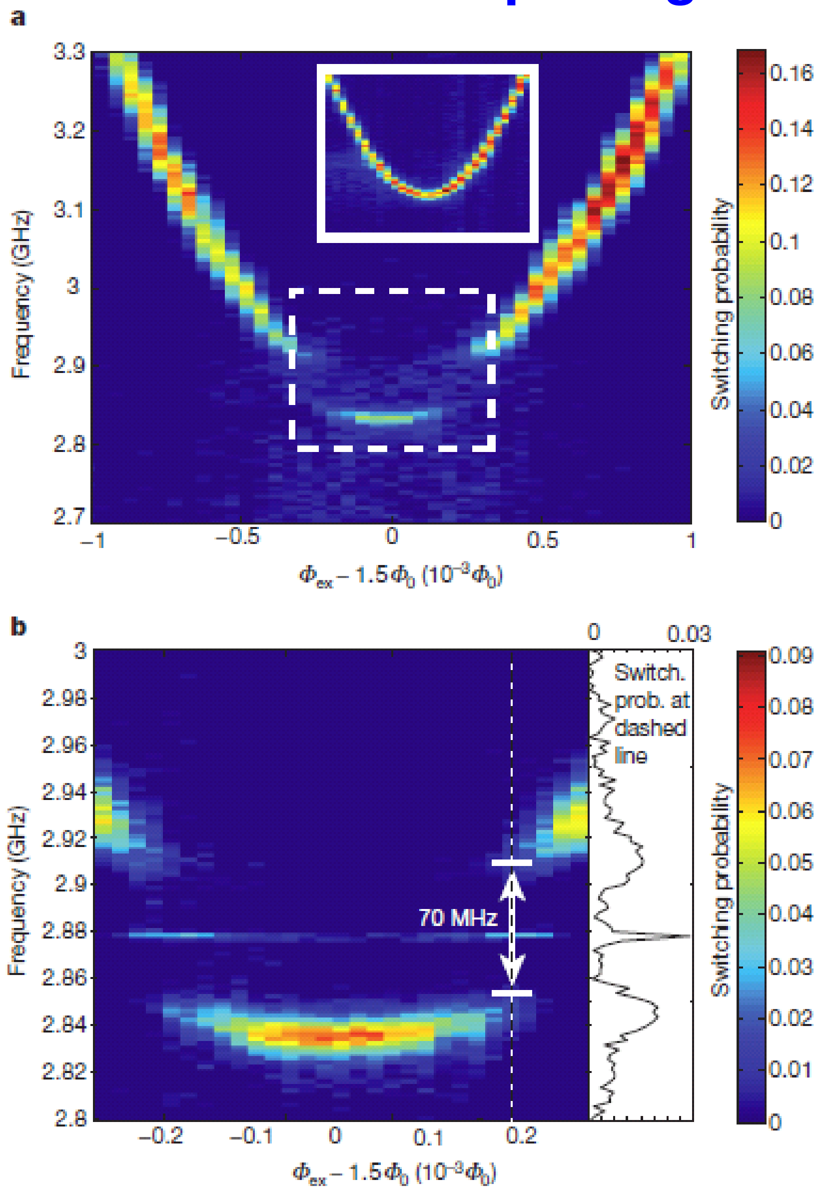
Kubo, PRL, 2010

Flux qubit

Arrangement

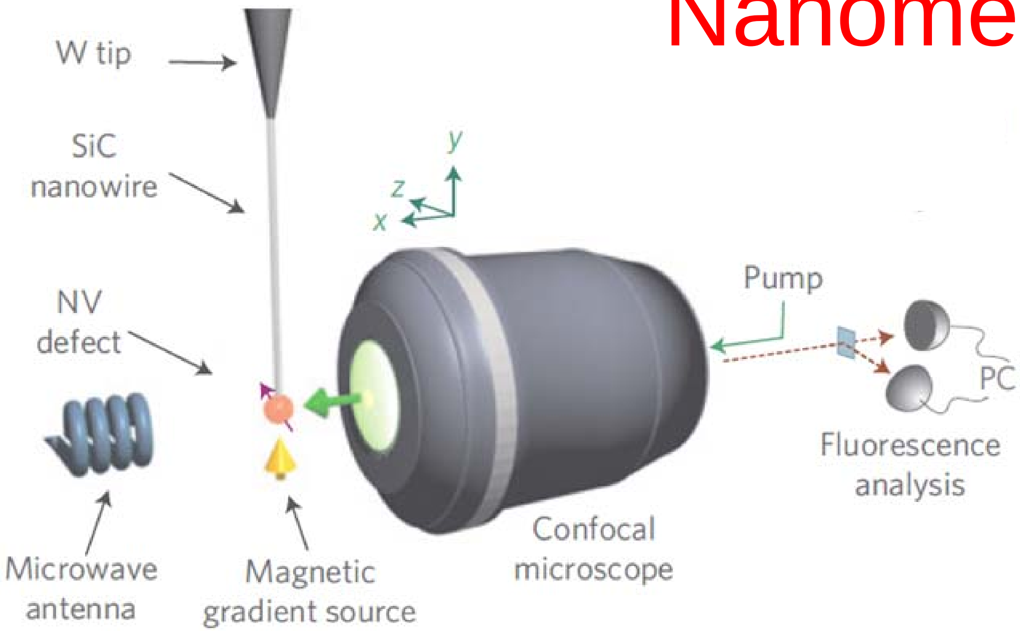


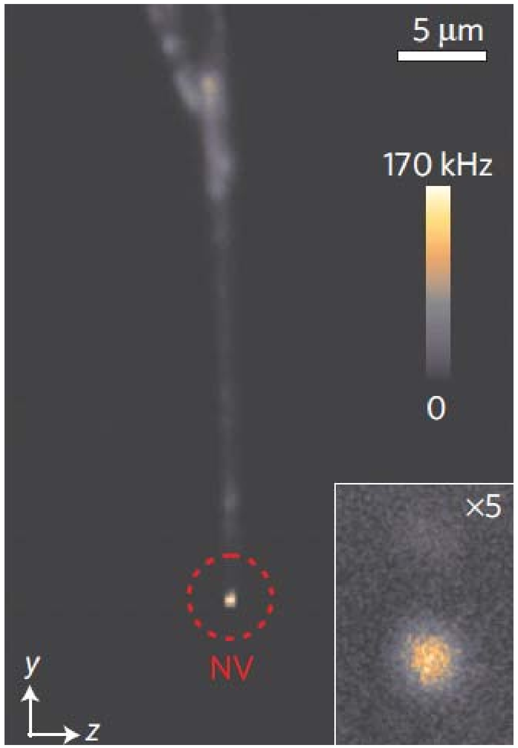
Vacuum Rabi splitting

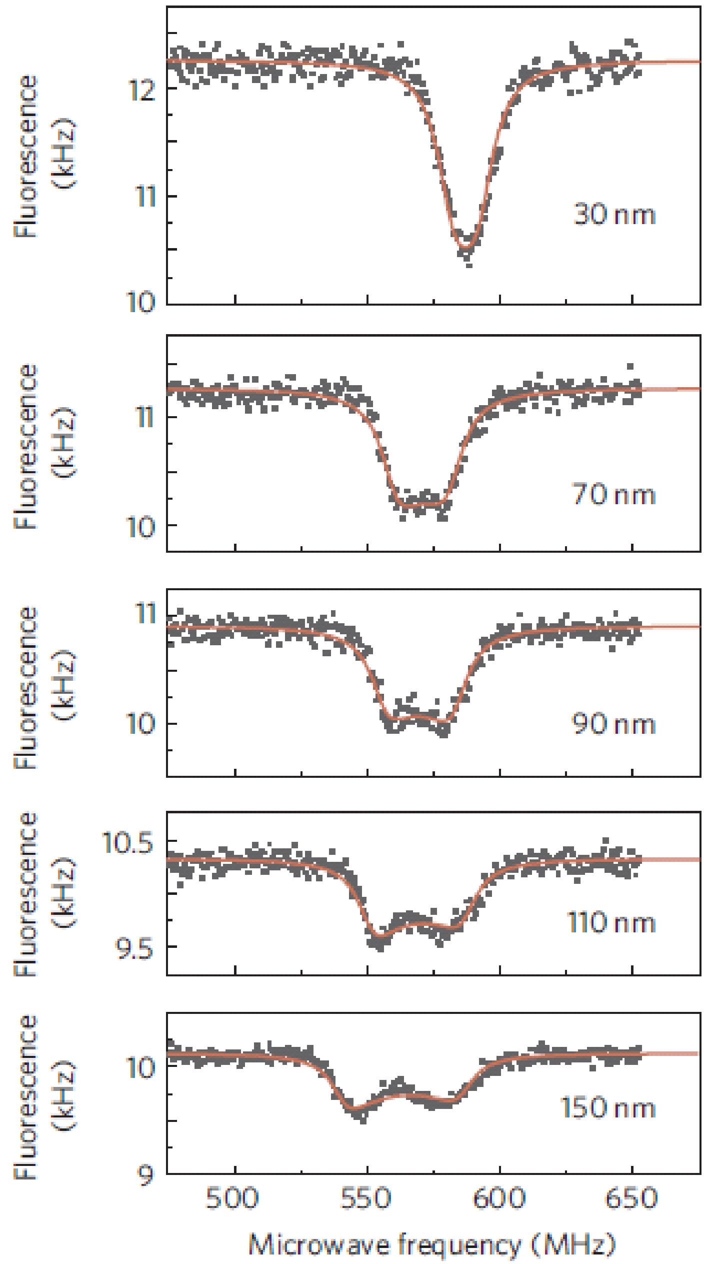


Semba, Nature, 2011

Nanomechanical resonators

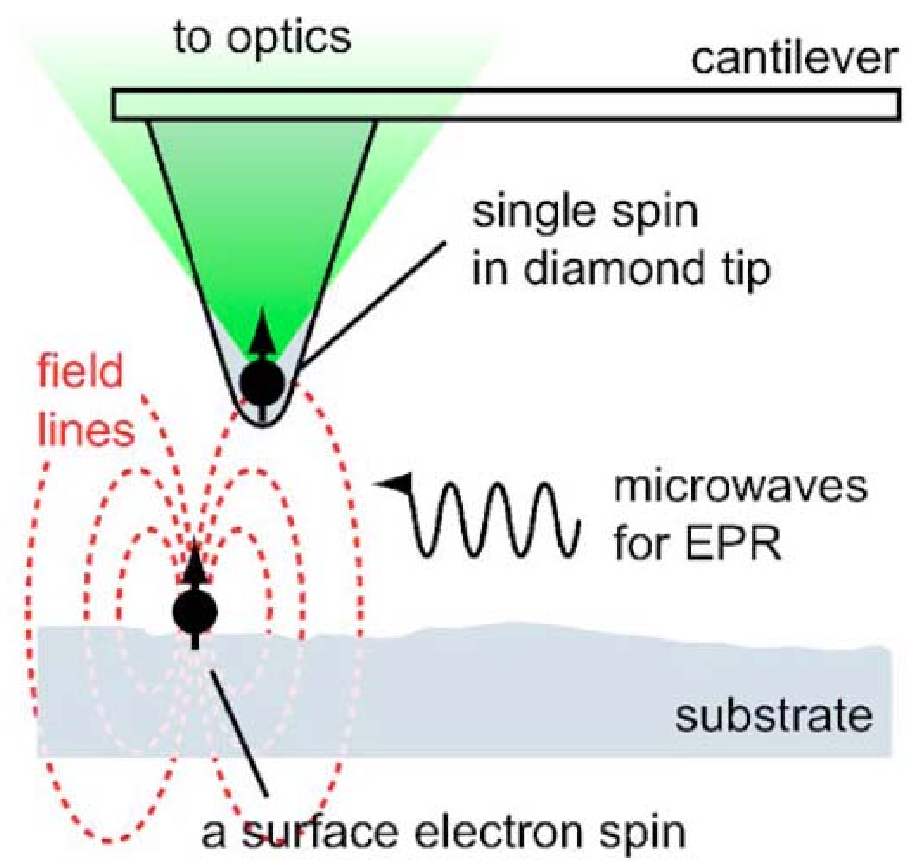






Arcizet, Nature Physics, 2011

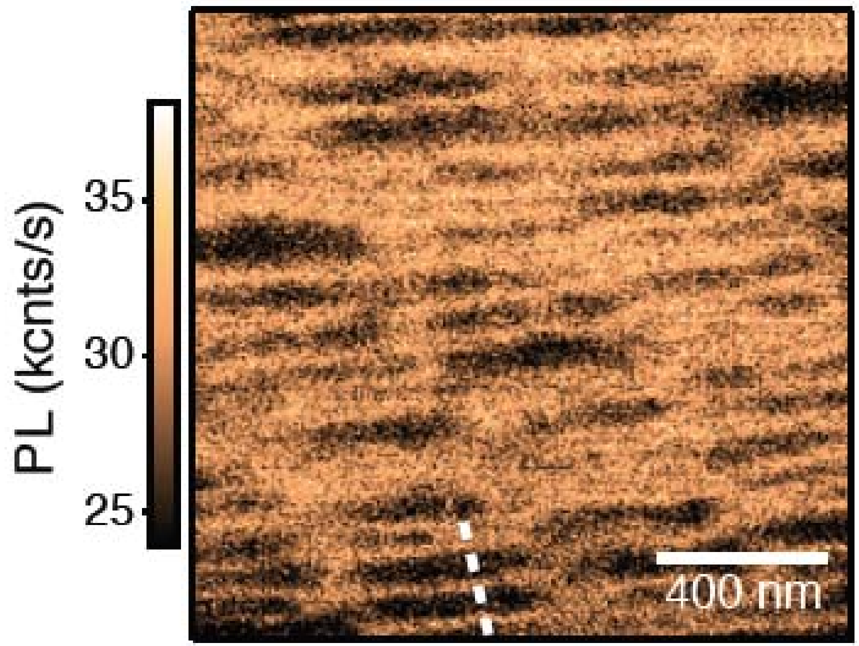
Application in nanoscale magnetic imaging



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)