自旋的量子控制与应用

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Outlines

- Introduction
- Quantum Computations
- Quantum Sensing

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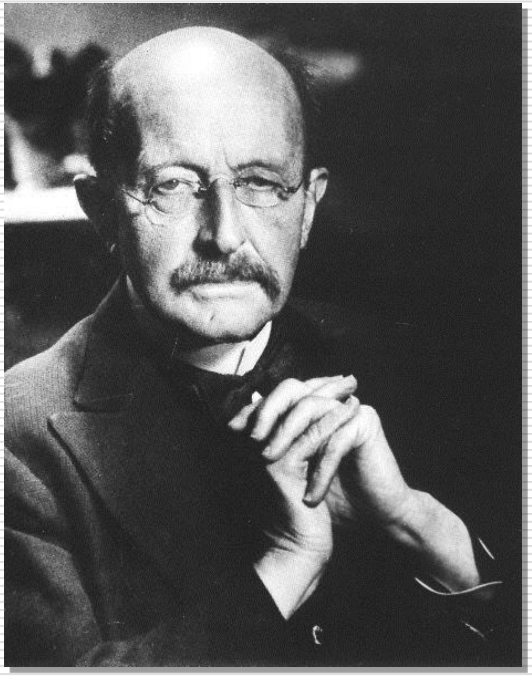
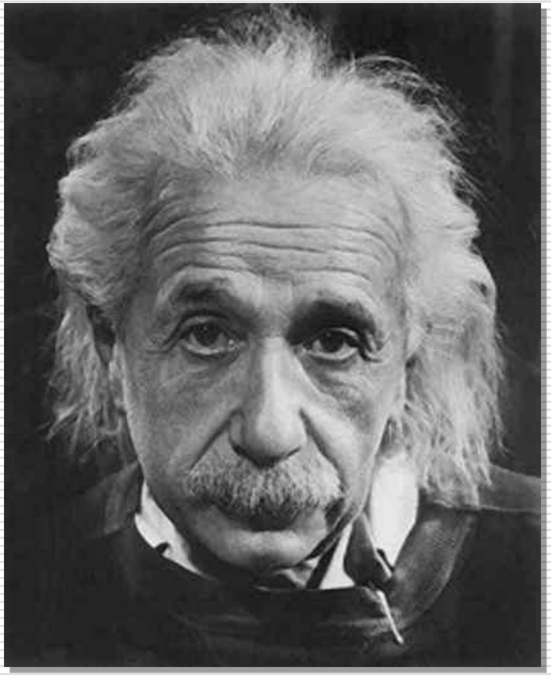
  - Background
  - Manipulation of spins
- Quantum Computations
- Quantum Sensing

Two greatest scientific discoveries in 20th century

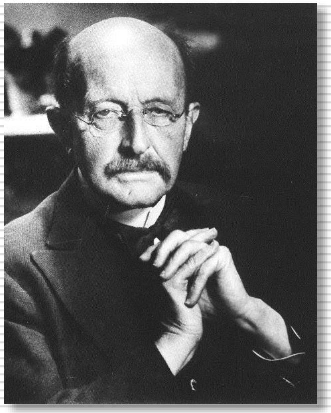


Max Planck
Quantum Theory
（1900）

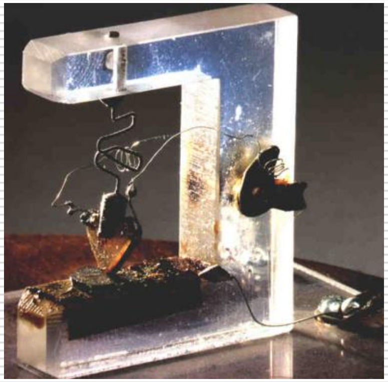


Albert Einstein
Theory of Relativity
（1905, 1915）

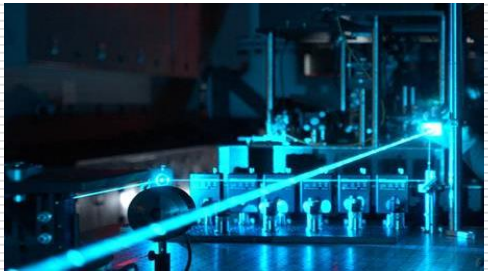
Quantum mechanics:
Pillar of modern physics and technologies



Energy quantization



Transistor



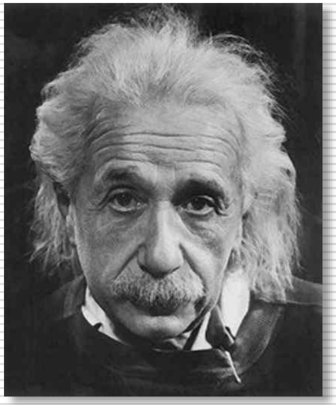
Laser

High-Tc superconductivity

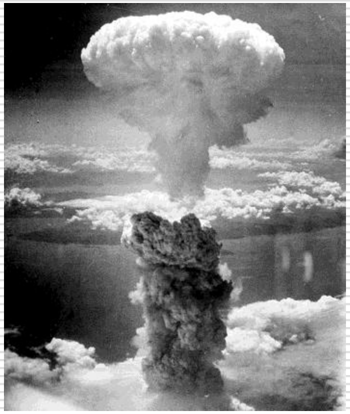
1895 1900 1905 1945 1947 1960 1973 1987 1988

X ray

Photoelectric effect



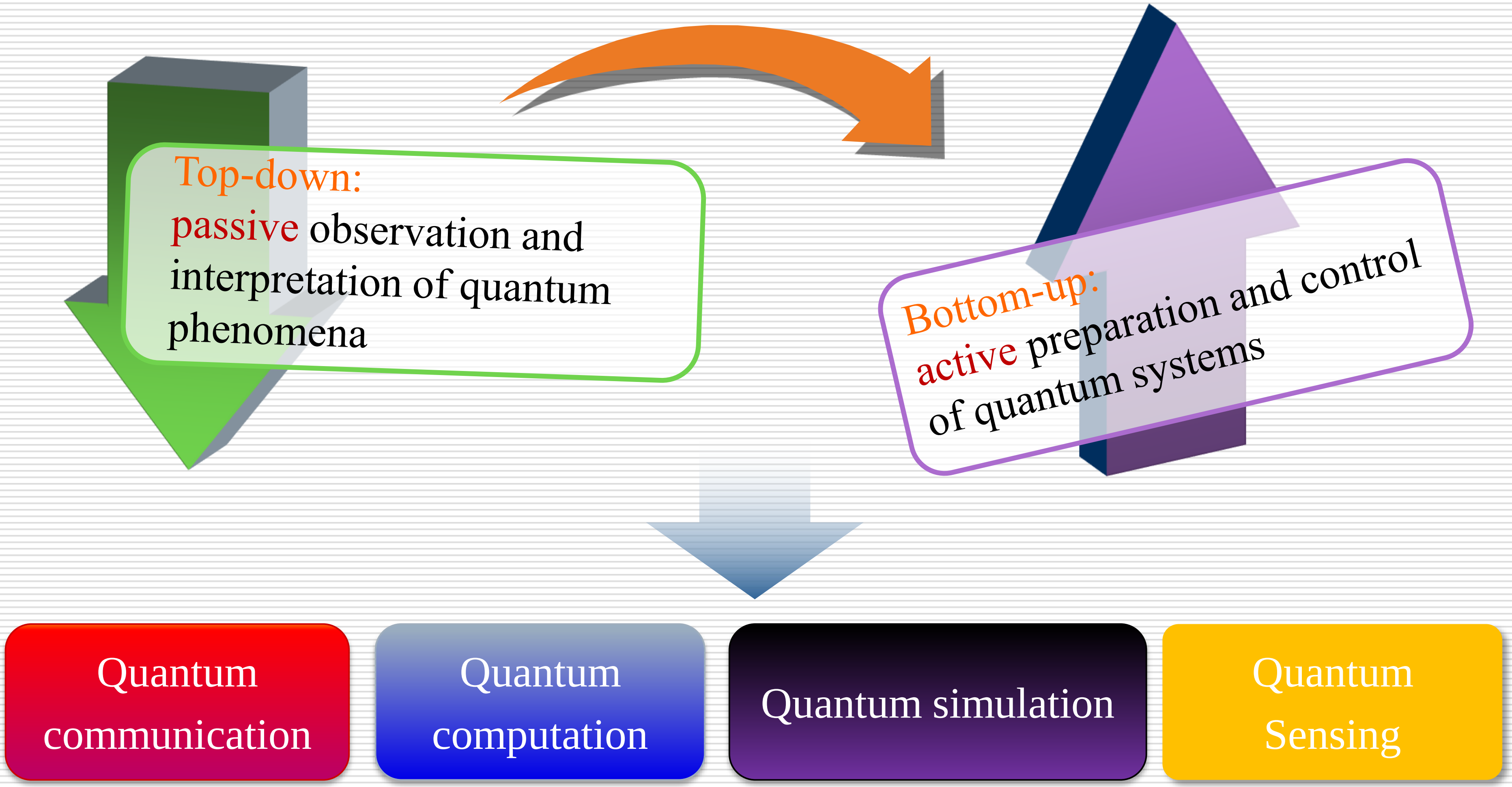
Atomic bomb



NMR

Giant magneto-resistance

Trends of quantum physics study



Top-down:
passive observation and interpretation of quantum phenomena

Bottom-up:
active preparation and control of quantum systems

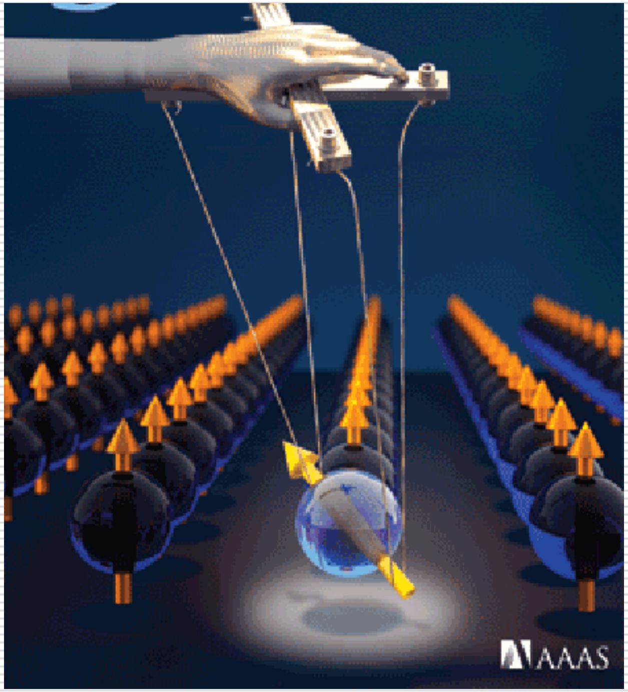
Quantum communication

Quantum computation

Quantum simulation

Quantum Sensing

Break the limits of classical technologies



Spatial scale: cm
Time scale: s
Frequency: ~10 Hz

Spatial scale: nm
Time scale: ns
Frequency: ~10^9 Hz

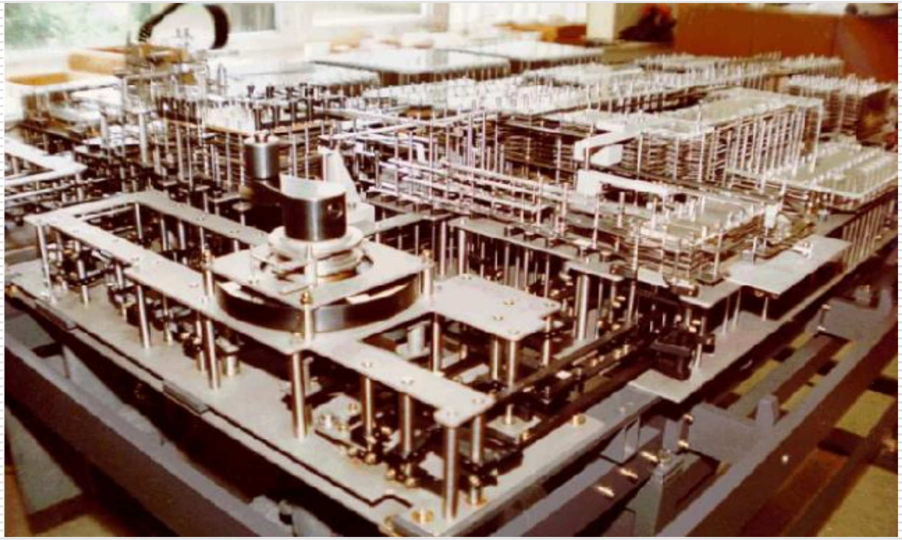
Outlines

- Introduction
- Quantum Computations
  - History of computing hardware
  - Basic principles of quantum computation
  - Physical implementation of quantum computation
- Quantum Sensing

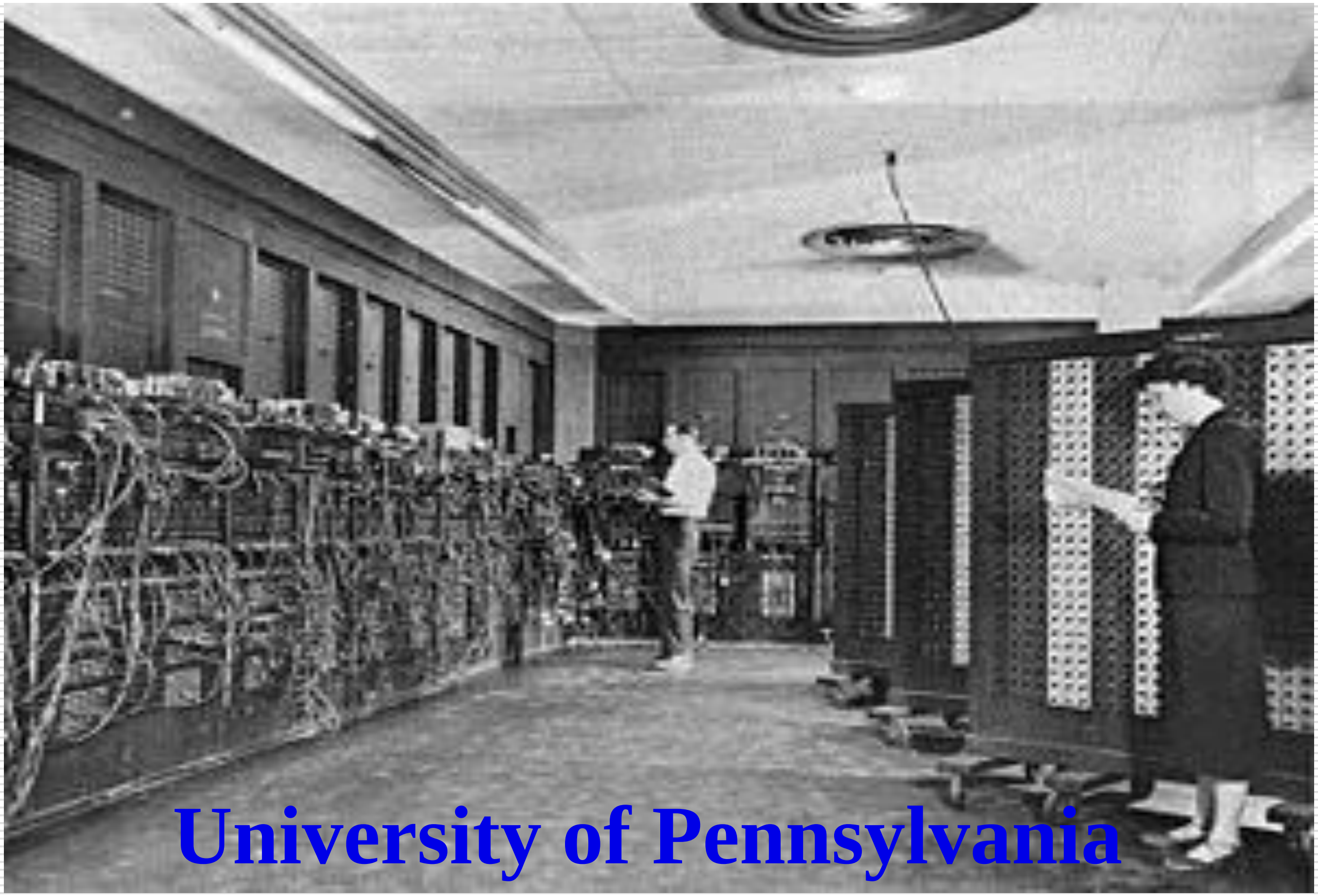
Development of classical computing

Mechanical, Abacus
13th century, China

Electromechanical
Programmable，
20th century, USA



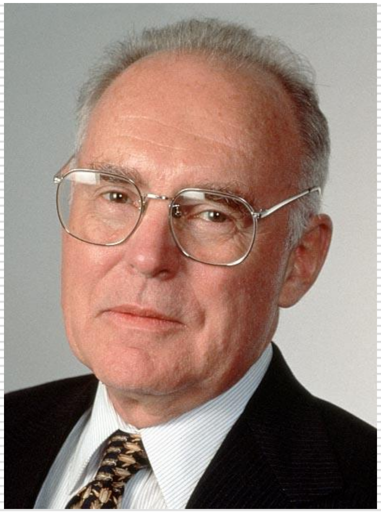
First electronic computer: 1946 ENIAC



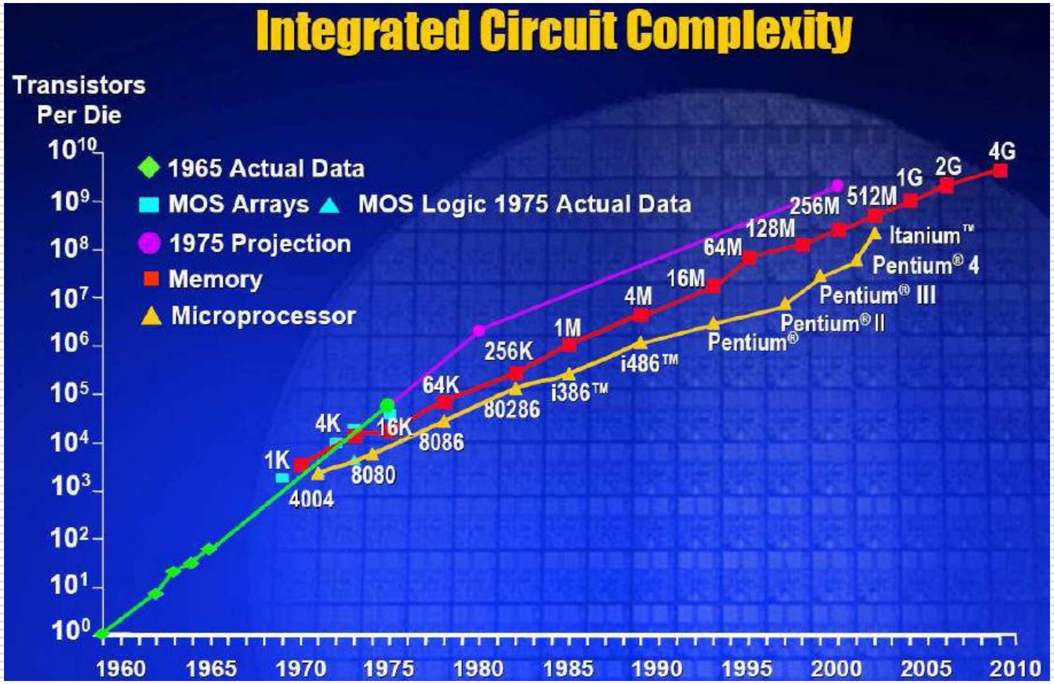
University of Pennsylvania

Moore's law

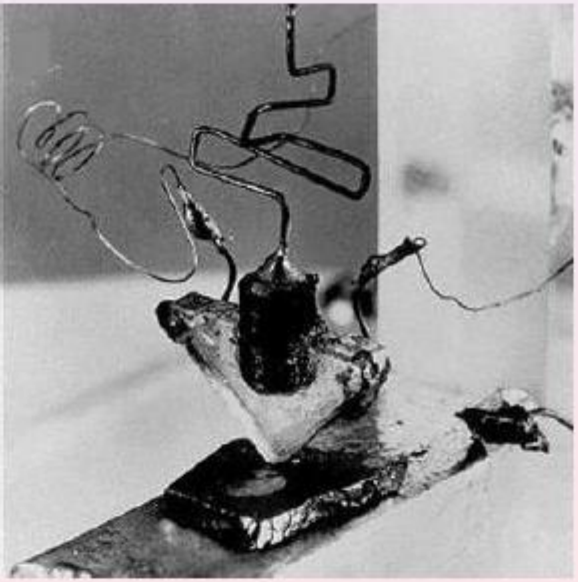
Moore‘s law is the observation that over the history of computing hardware, the number of transistors on integrated circuits doubles approximately every 18 months.



Gordon E. Moore
(Intel 1965)

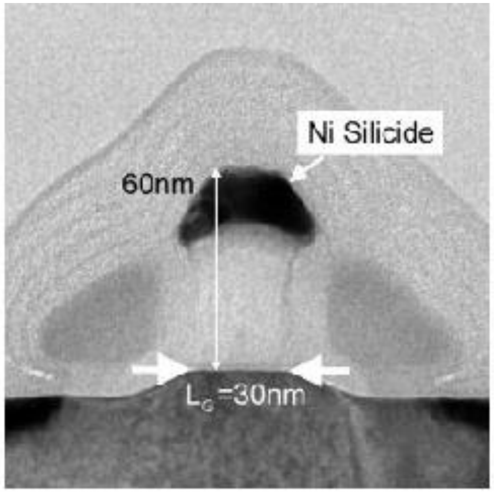


Getting Smaller



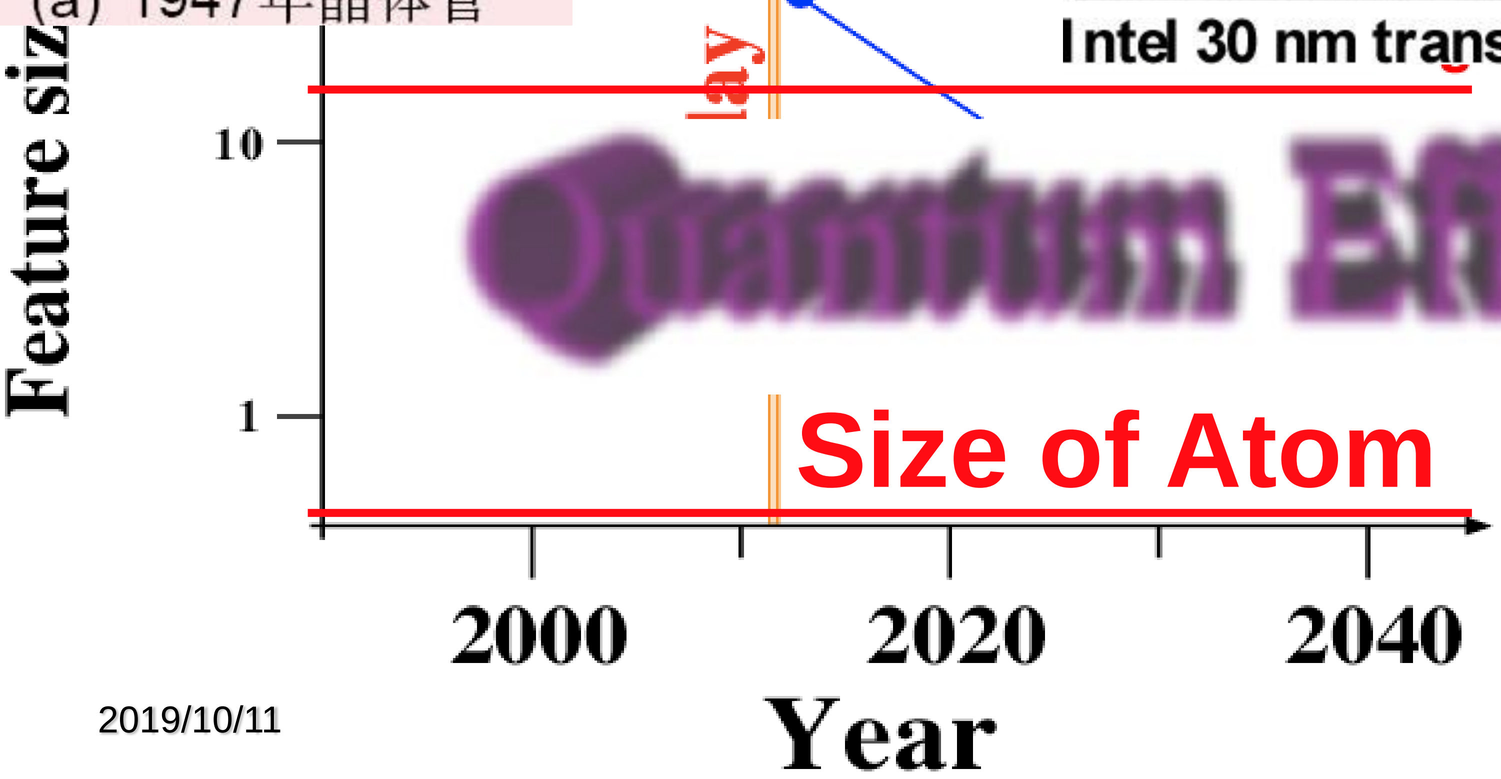
(a) 1947年晶体管

Semico ry
Associa



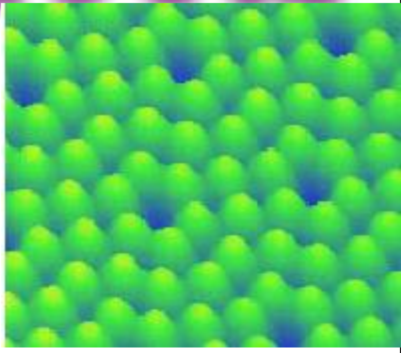
Intel 30 nm transistor

lectron

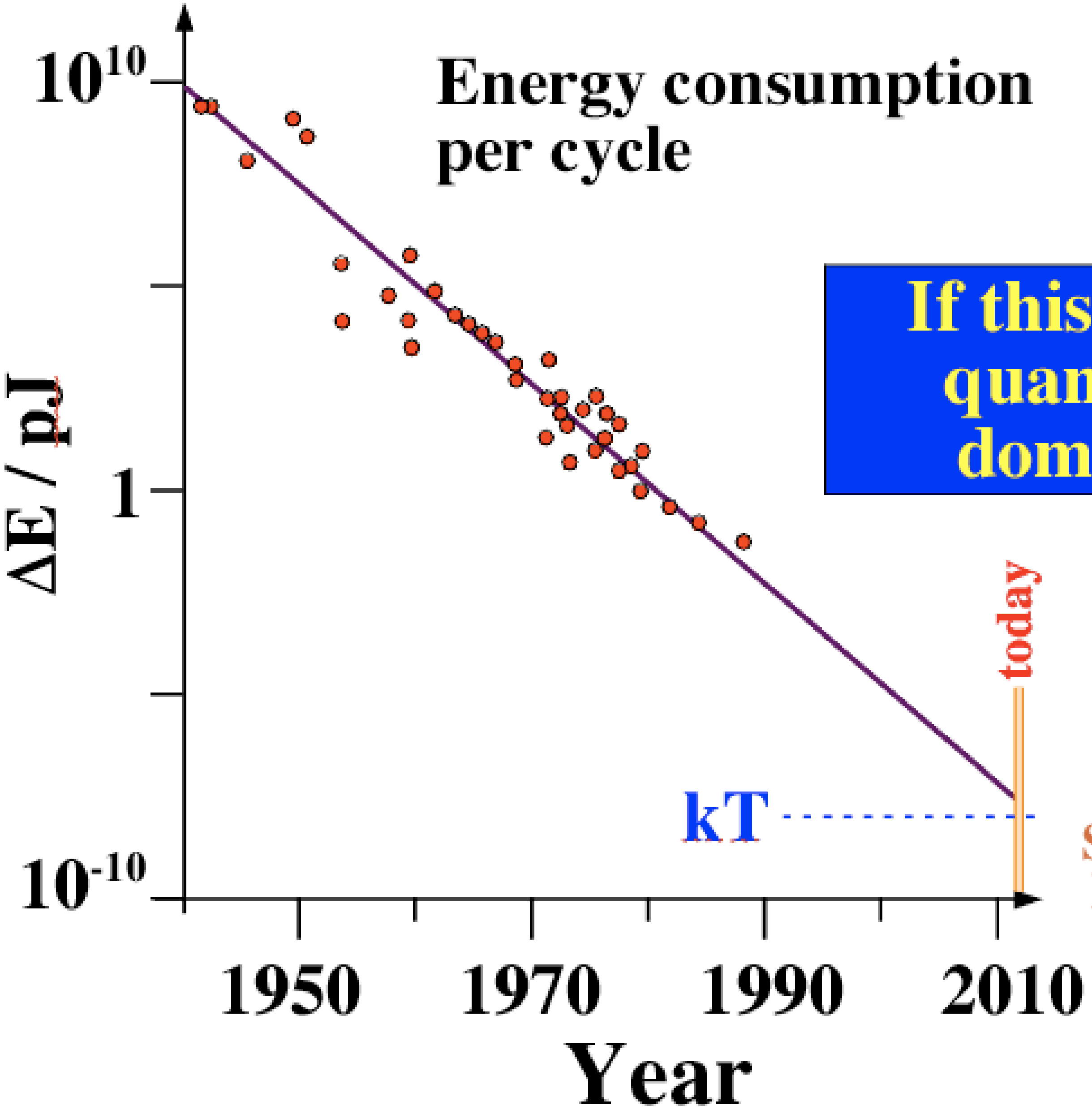


Quantum Effects

Size of Atom



Cooler Computers



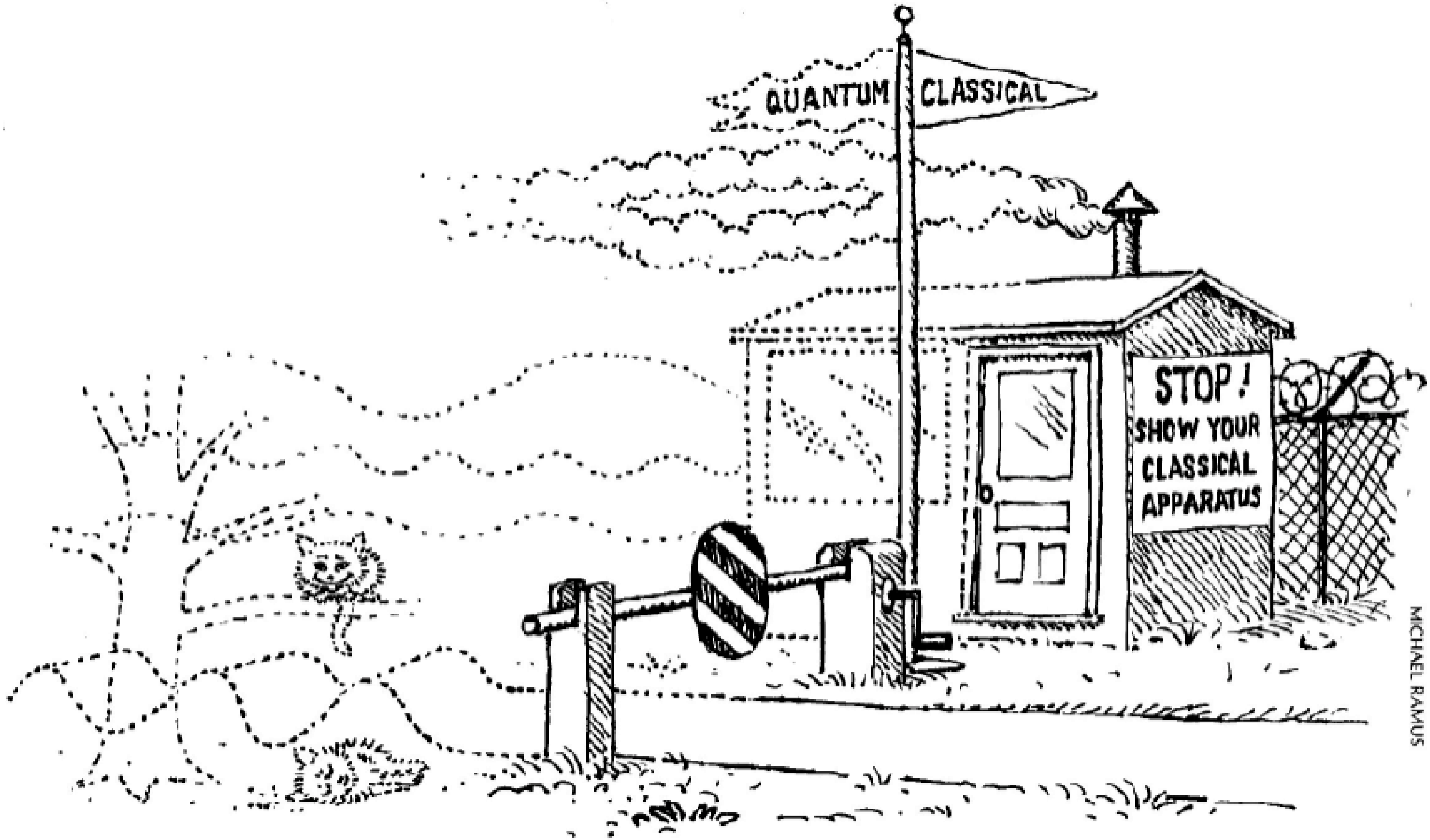
If this trend continues, quantum effects will dominate very soon

"Brownian Motion"

Switches become unstable

Minimum dissipation for boolean logic

Electronics at the Quantum - Classical Border

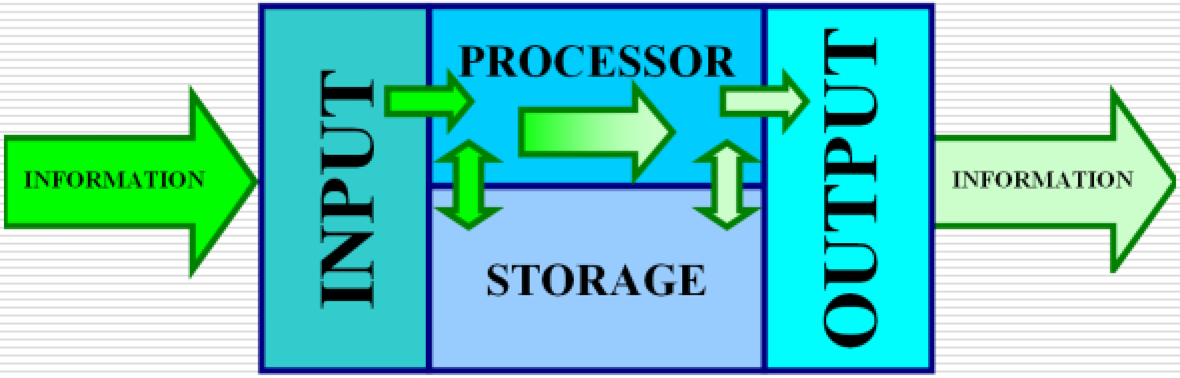


W. Zurek, "Decoherence and the transition from quantum to classical, Physics Today, October 1991.

What is Quantum Computation?

Quantum Computer

Quantum computations performs calculations based on *<u>the laws of quantum mechanics</u>*, which is the behavior of particles at the *<u>sub-atomic level</u>*.



INFORMATION

INPUT

PROCESSOR

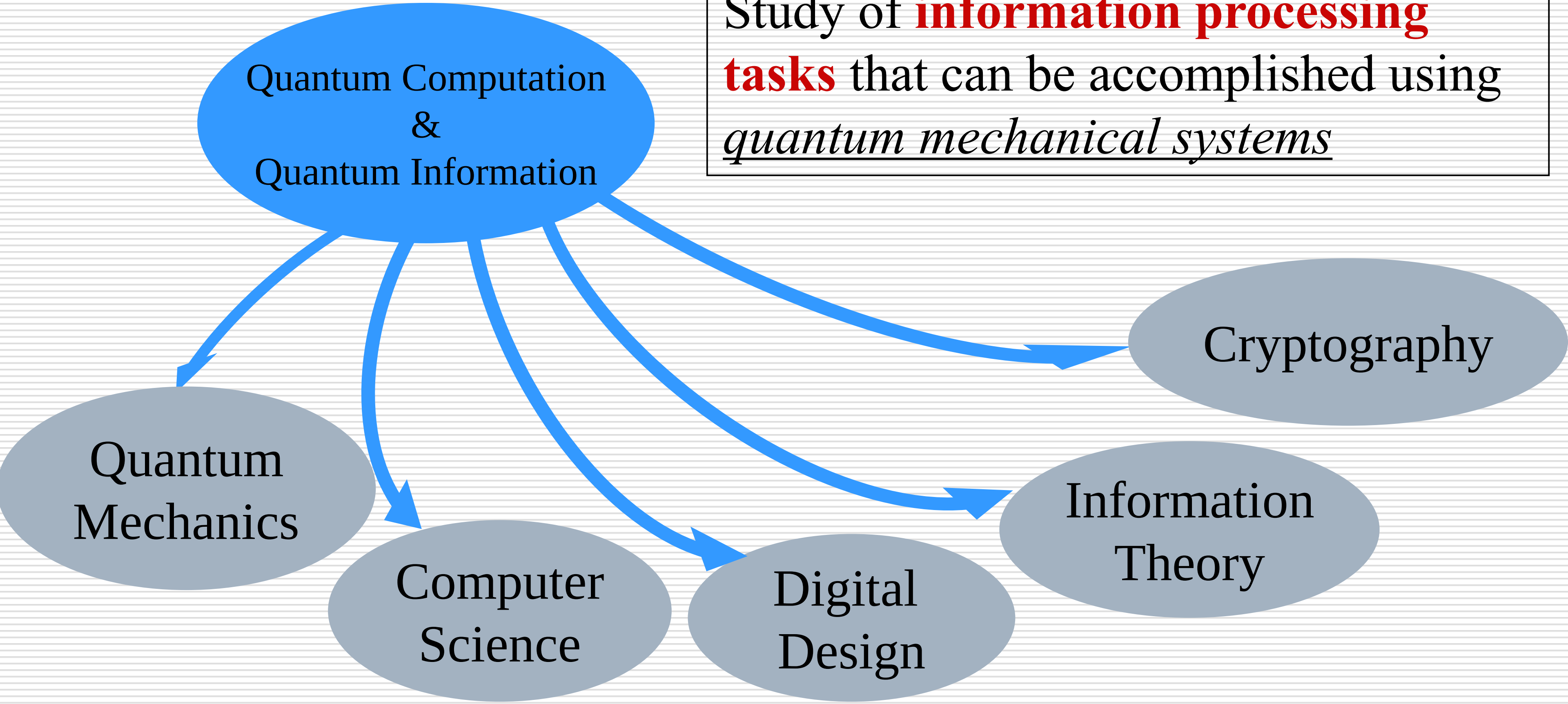
STORAGE

OUTPUT

INFORMATION

Quantum Computations

Study of **information processing tasks** that can be accomplished using *quantum mechanical systems*



Quantum Computation
&
Quantum Information

Quantum Mechanics

Computer Science

Digital Design

Information Theory

Cryptography

Data representation

classical

2 possible voltages
encode one bit

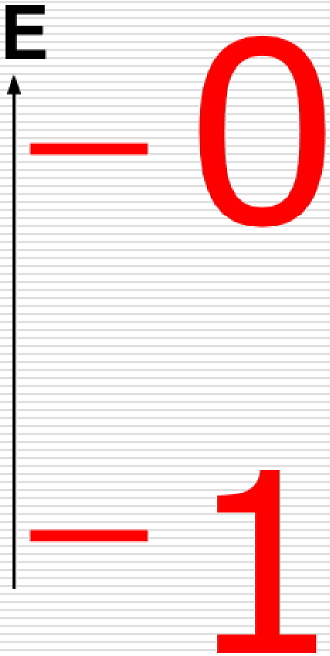
0

or

1

quantum mechanical

2-level system
encodes one bit



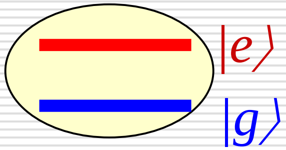
or

"Qubit"

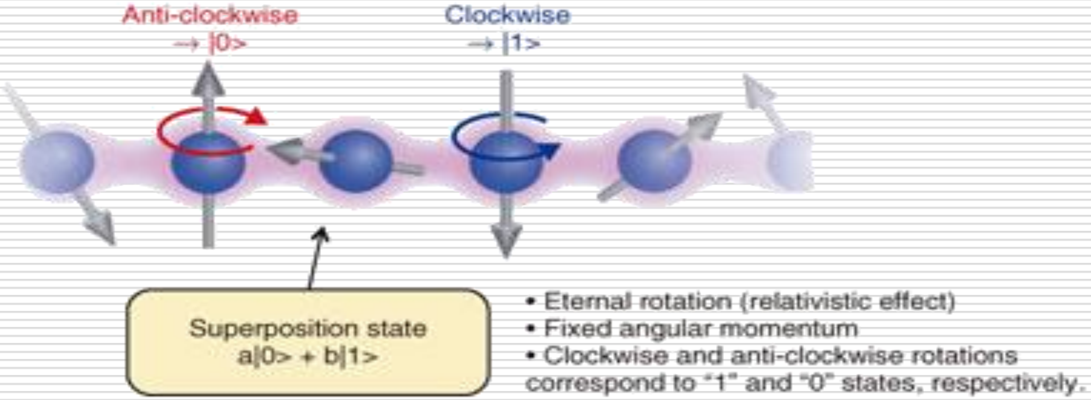
Implementation of Qubits

Photon Polarization encoding (|Horizontal> and |Vertical>)
Fock state (| Vacuum> and |Single photon>

Two-level atom



Spin



- Eternal rotation (relativistic effect)
- Fixed angular momentum
- Clockwise and anti-clockwise rotations correspond to "1" and "0" states, respectively.

Classical operation v.s. Quantum operation

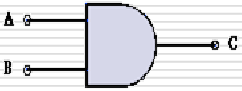
Classical Boolean Logic
(irreversible)

Quantum Logic
(reversible)

Example 1: **NOT**

Input **Output**

$$\left.\begin{matrix}0\\1\end{matrix}\right\} \rightarrow \left\{\begin{matrix}1\\0\end{matrix}\right.$$



Example 2: **AND**

Input **Output**

$$\left.\begin{matrix}0\ 0\\0\ 1\\1\ 0\\1\ 1\end{matrix}\right\} \rightarrow \left\{\begin{matrix}0\\0\\0\\1\end{matrix}\right.$$

AND gate loses information

↓

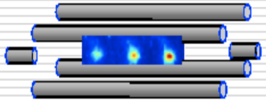
Minimal energy dissipation : kT ln2

↓

not available in QIP

Logical operation :

$$\Psi_{out} = U\,\Psi_{in}$$

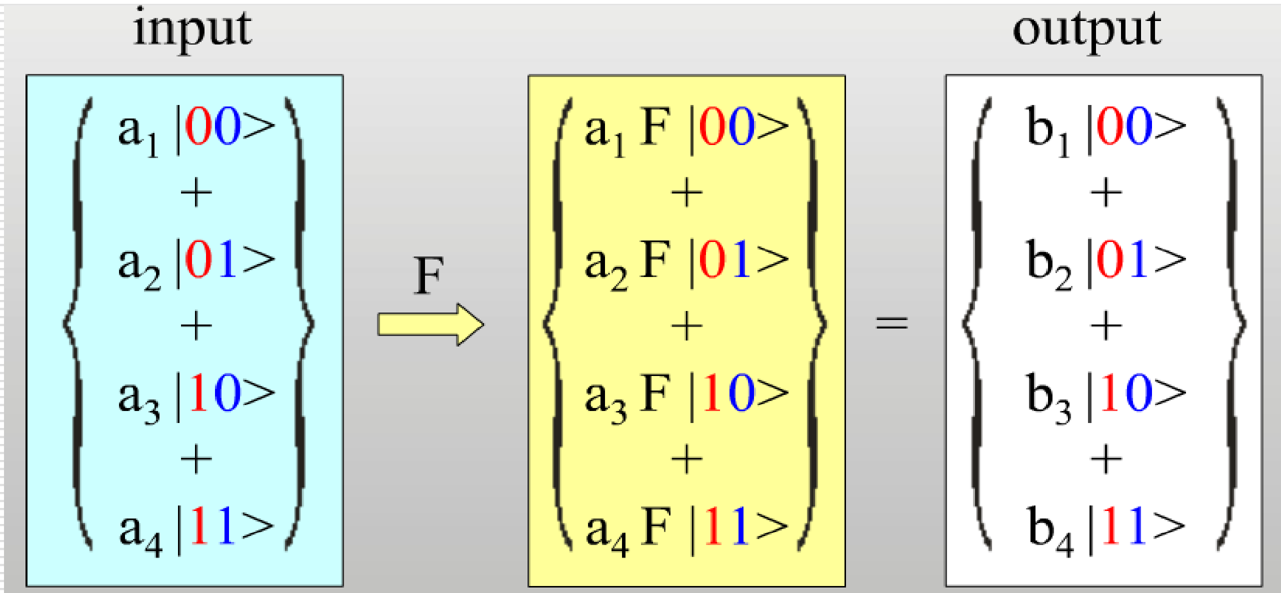


- Quantum logical operations are reversible: $\Psi_{in} = U^{-1}\,\Psi_{out}$
- No dissipation

Time evolution driven by Hamiltonian

$$U = T\int e^{-i\mathcal{H}(t)}\,dt = e^{-iH_{eff}\tau}$$

Quantum parallelism



$$\begin{Bmatrix} a_1\,|00> \\ + \\ a_2\,|01> \\ + \\ a_3\,|10> \\ + \\ a_4\,|11> \end{Bmatrix} \xrightarrow{F} \begin{Bmatrix} a_1\,F\,|00> \\ + \\ a_2\,F\,|01> \\ + \\ a_3\,F\,|10> \\ + \\ a_4\,F\,|11> \end{Bmatrix} = \begin{Bmatrix} b_1\,|00> \\ + \\ b_2\,|01> \\ + \\ b_3\,|10> \\ + \\ b_4\,|11> \end{Bmatrix}$$

- Superposition for input created by Hadamard gates
- Functions are represented by unitary operators
- Quantum state tomography – but how to get a “real” result?

Classical vs. Quantum

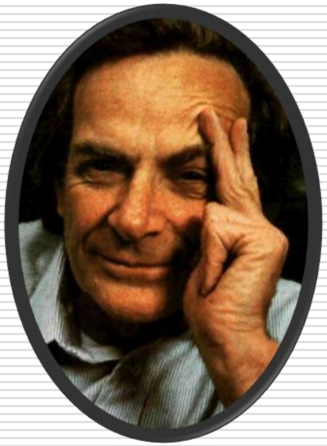
Rules on Data	Classical	Quantum
Representation	0 or 1	0 or 1 and inbetween
Operations	Boolean logic irreversible	Quantum logic Unitary, reversible
Measurements	Deterministic	Undeterministic Projection measurement

Quantum computations: compute differently

New model of computation can be faster than its classical counterpart.

Quantum algorithms

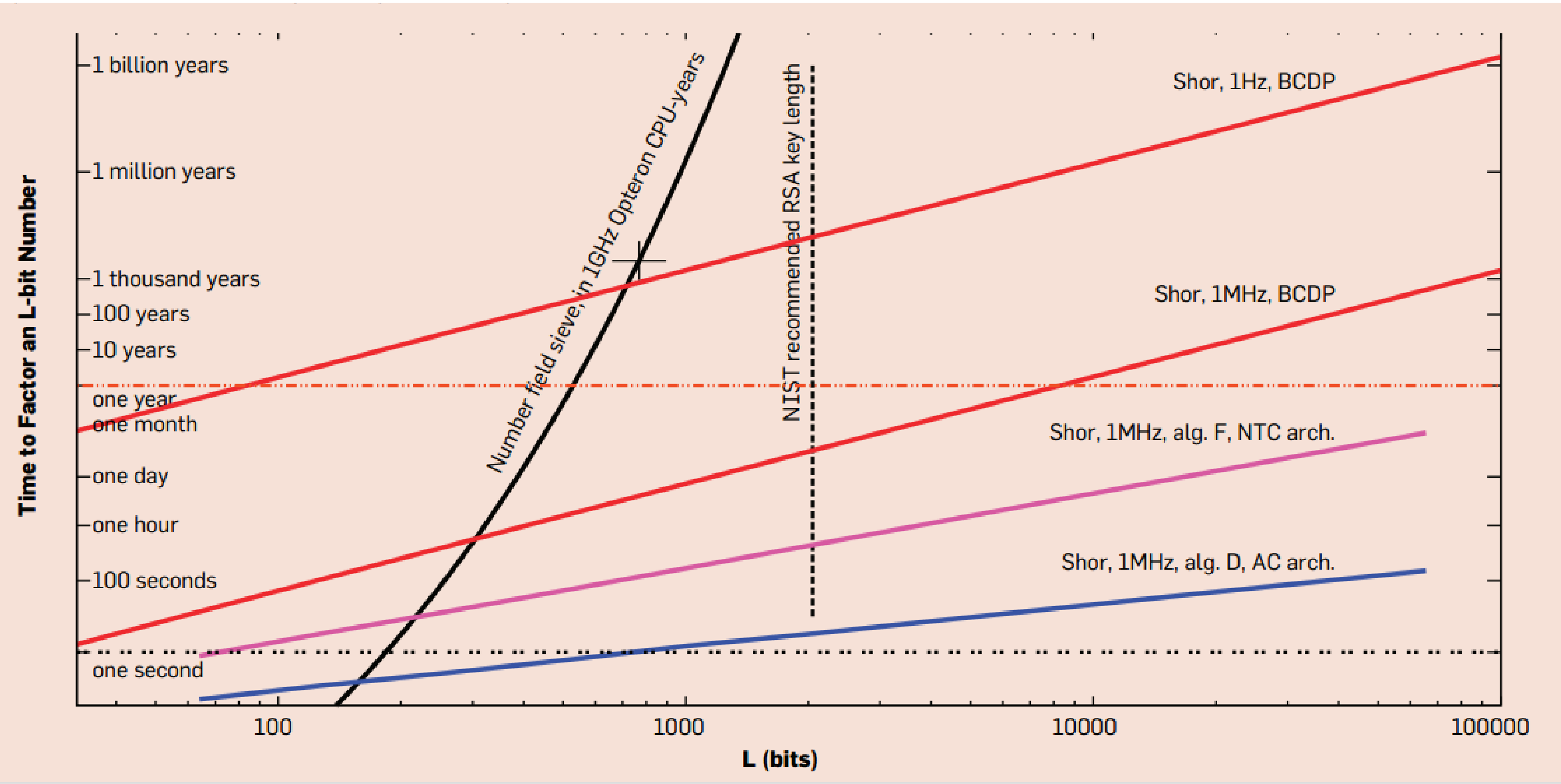
Solve some Hard classical problems



Quantum simulations

A medium-scale quantum simulation with 30 to 100 qubits can exceed the limitations of classical computing!

Classical algorithm v.s. Quantum algorithm



Physical implementation of QC

DiVincenzo's 5 criteria

- Well-defined qubits
- Initialization to a pure state
- Long coherence times
- Universal set of quantum gates
- Qubit-specific measurement

DiVincenzo D.P., Fortschr. Physik, 48 (9-11), 771 – 783 (2000)
The Physical Implementation of Quantum Computation

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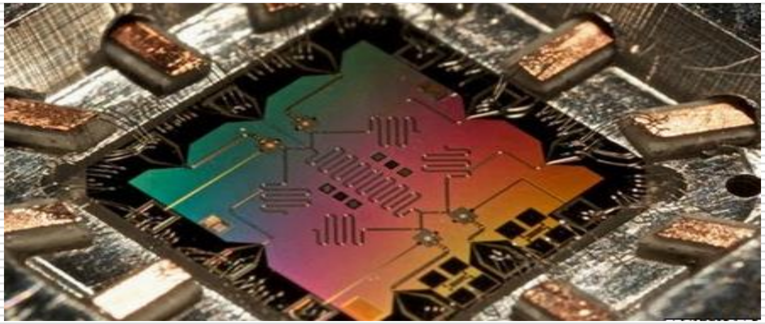
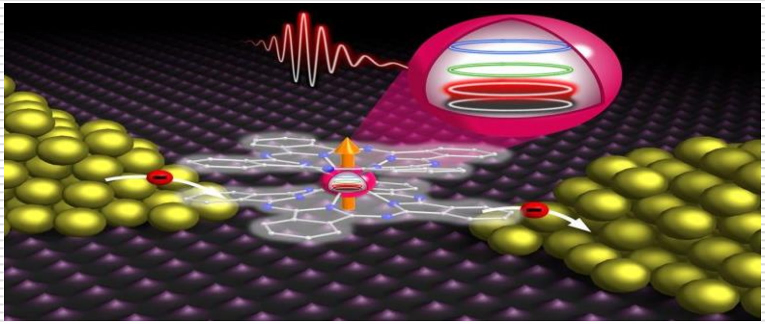
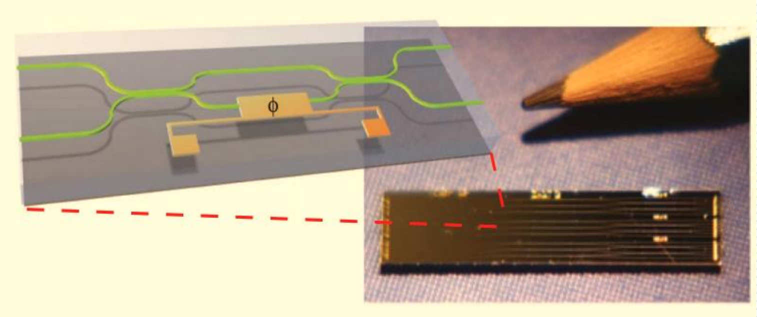
Physical systems for QC



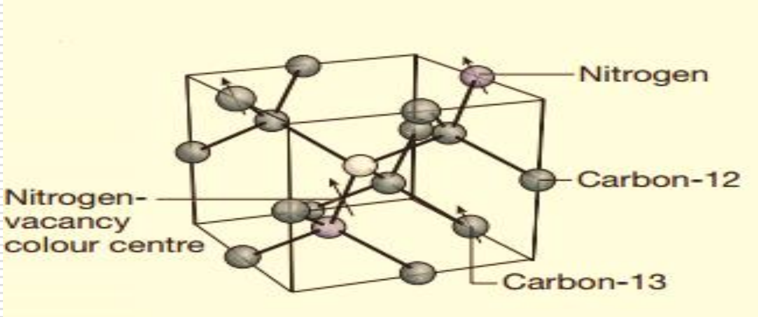
Superconducting Qubit



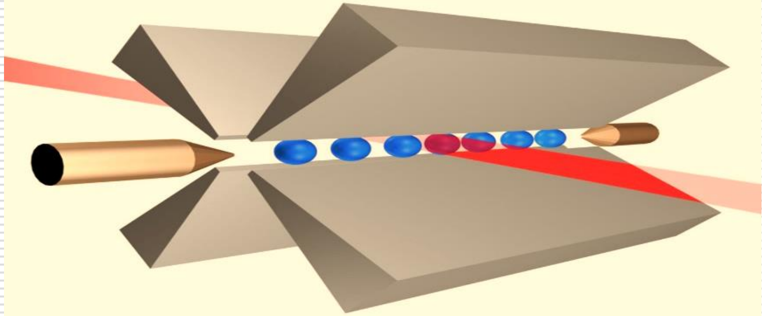
Single molecule magnet



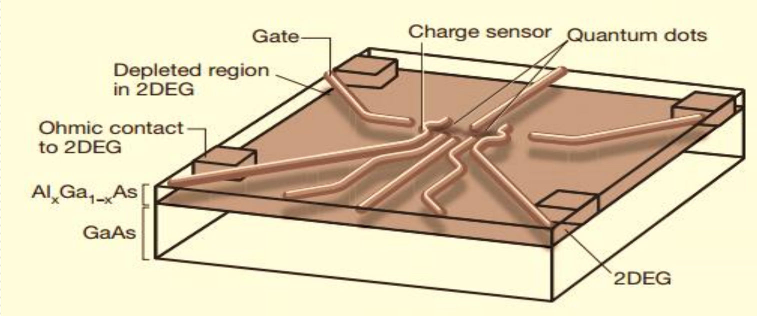
Photon



NV centers in diamons



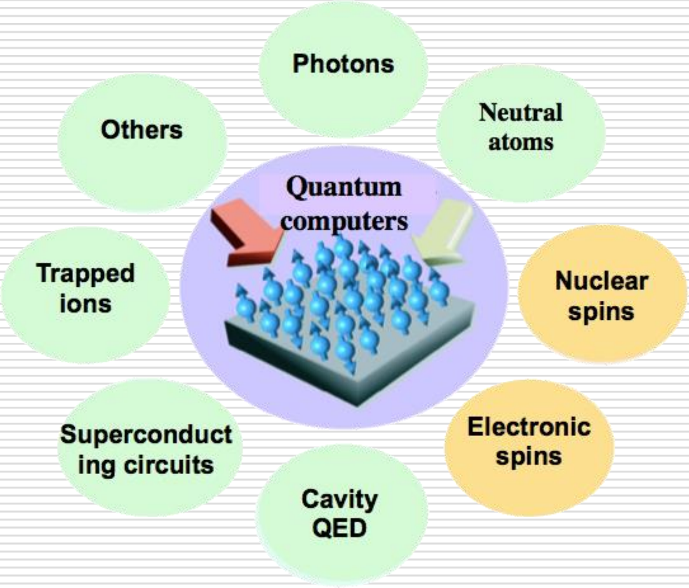
Trapped ions



Quantum dots

Pictures from **Nature** 464, 45 (2010) and **Science** 344, 1135 (2014)

Spin-based quantum computations

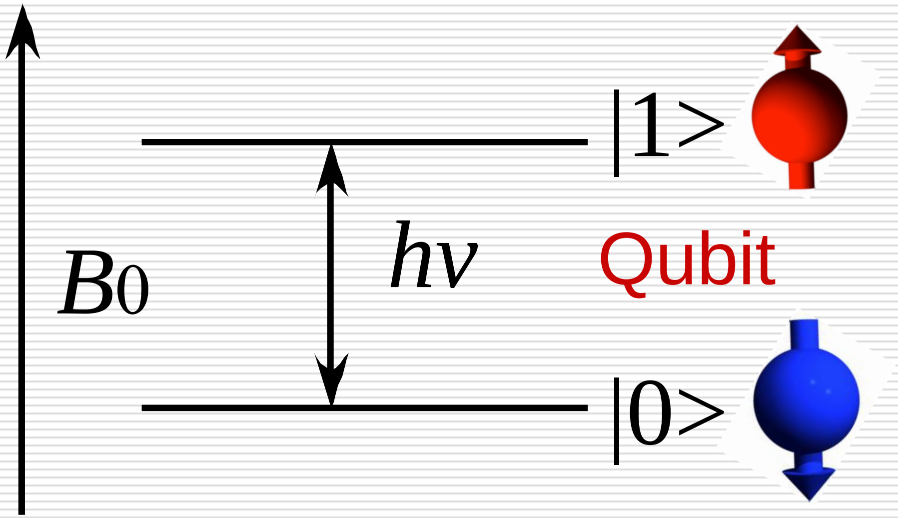


- **Nuclear spins have long decoherence time**
- **Electronic spins have the fast operation time**
- **Spins can be easily manipulated by mature magnetic resonance techniques (NMR, EMR, ODMR, FMR)**

Spin-based QC is one of most successful physical implementations, and provides inspired technology for others solid systems, as an important testbed for developing quantum control methods.

Manipulation of spins:
Various spin magnetic resonance techniques

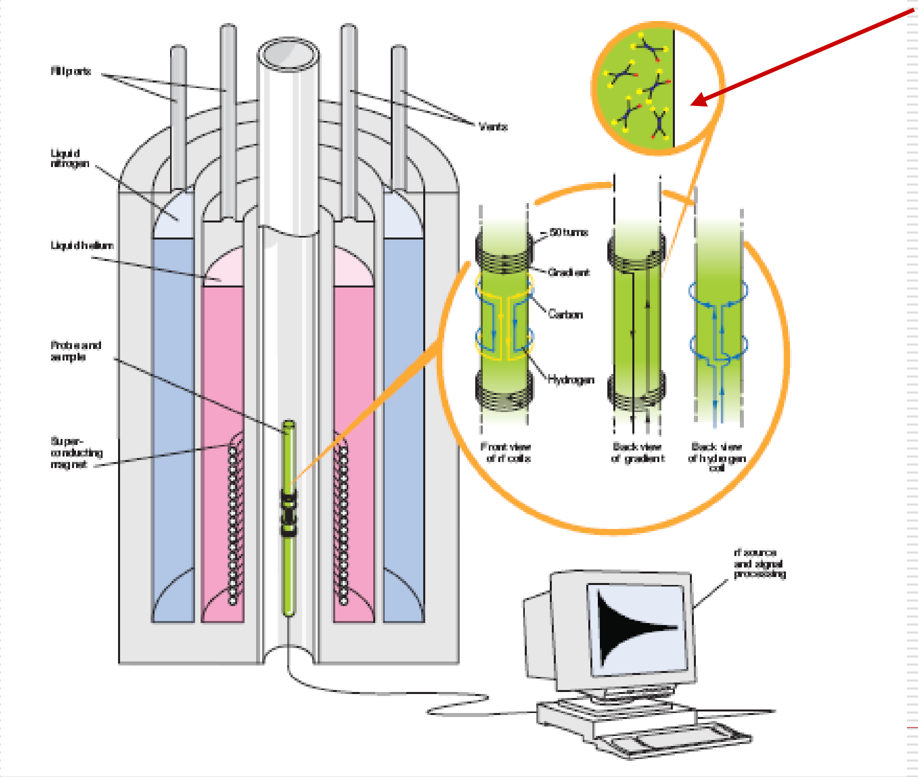
Spin 1/2 particle in magnetic field



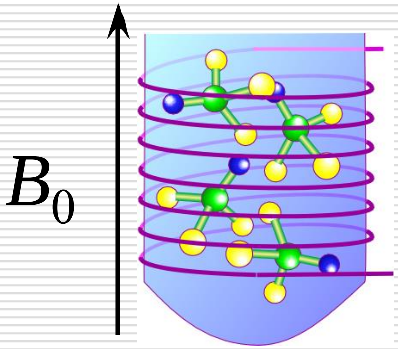
Frequency	Technique
PHz (10^{12})	ODMR
GHz (10^{9})	ESR
MHz (10^{6})	NMR
kHz (10^{3})	FMR

Nuclear magnetic resonance (NMR)

Liquid state NMR is an excellent system for small quantum registers.



NMR quantum register



Control：
Radiofrequency pulses
Spin-spin interactions

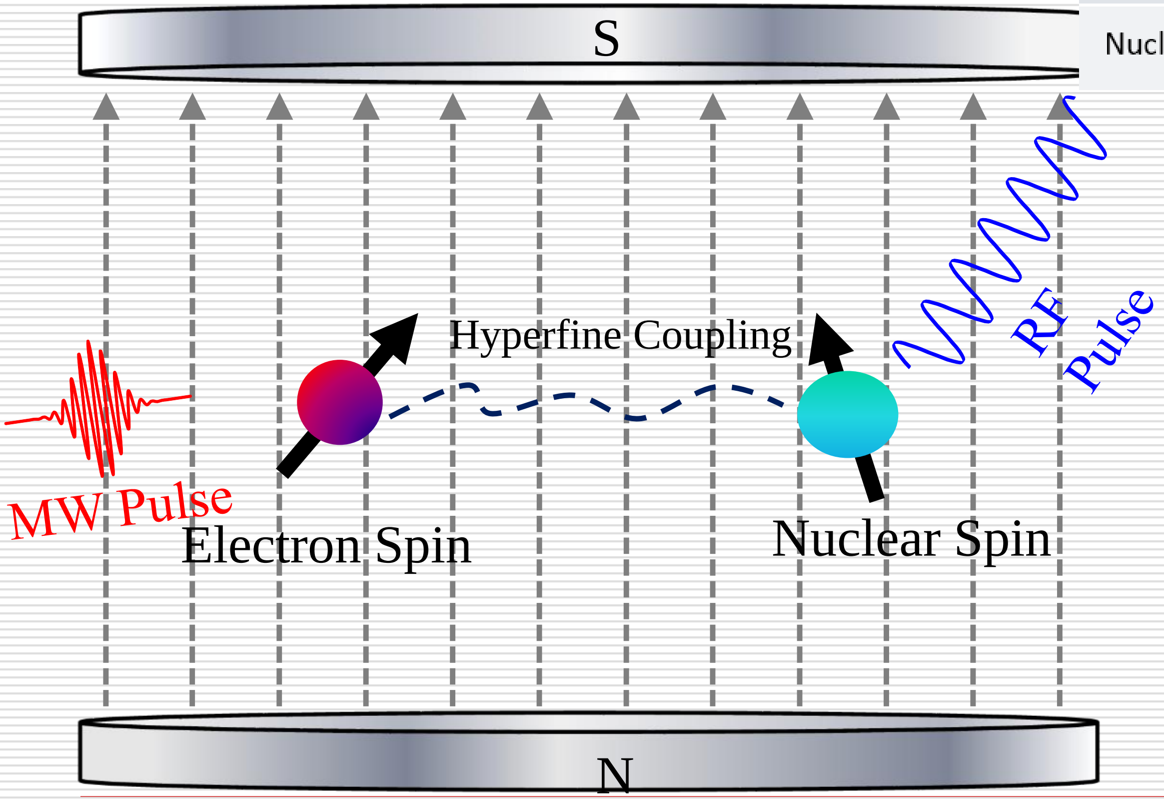
Initialization：Pseudo-pure state

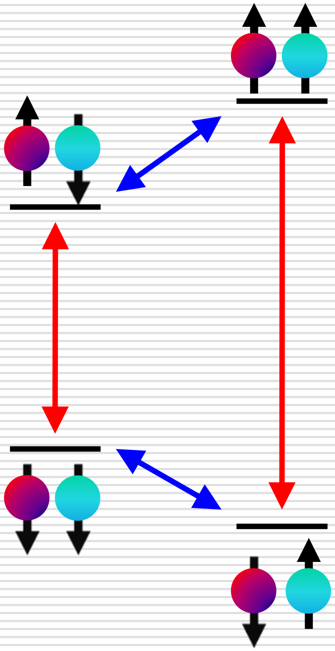
Readout: Ensemble

Electron spin resonance (ESR)

ESR: manipulation of the electron spins and the nuclear spins.

	Manipulation rate	**Coherence time**
Electron spin	Fast	short
Nuclear spin	Slow	Long





Optically detected magnetic resonance (ODMR)

NV center in diamond

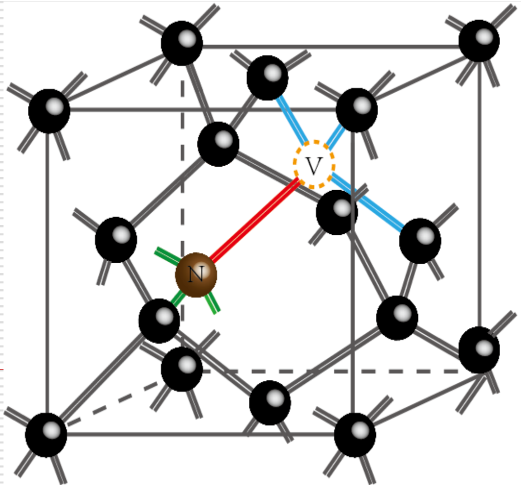
Optics:
initialize and readout

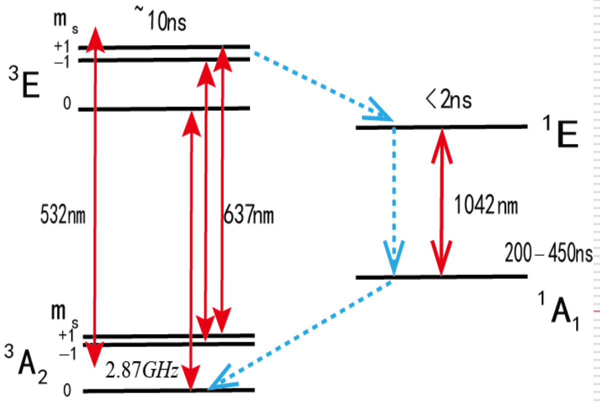
(Quantum communication)

Microwave:
manipulation

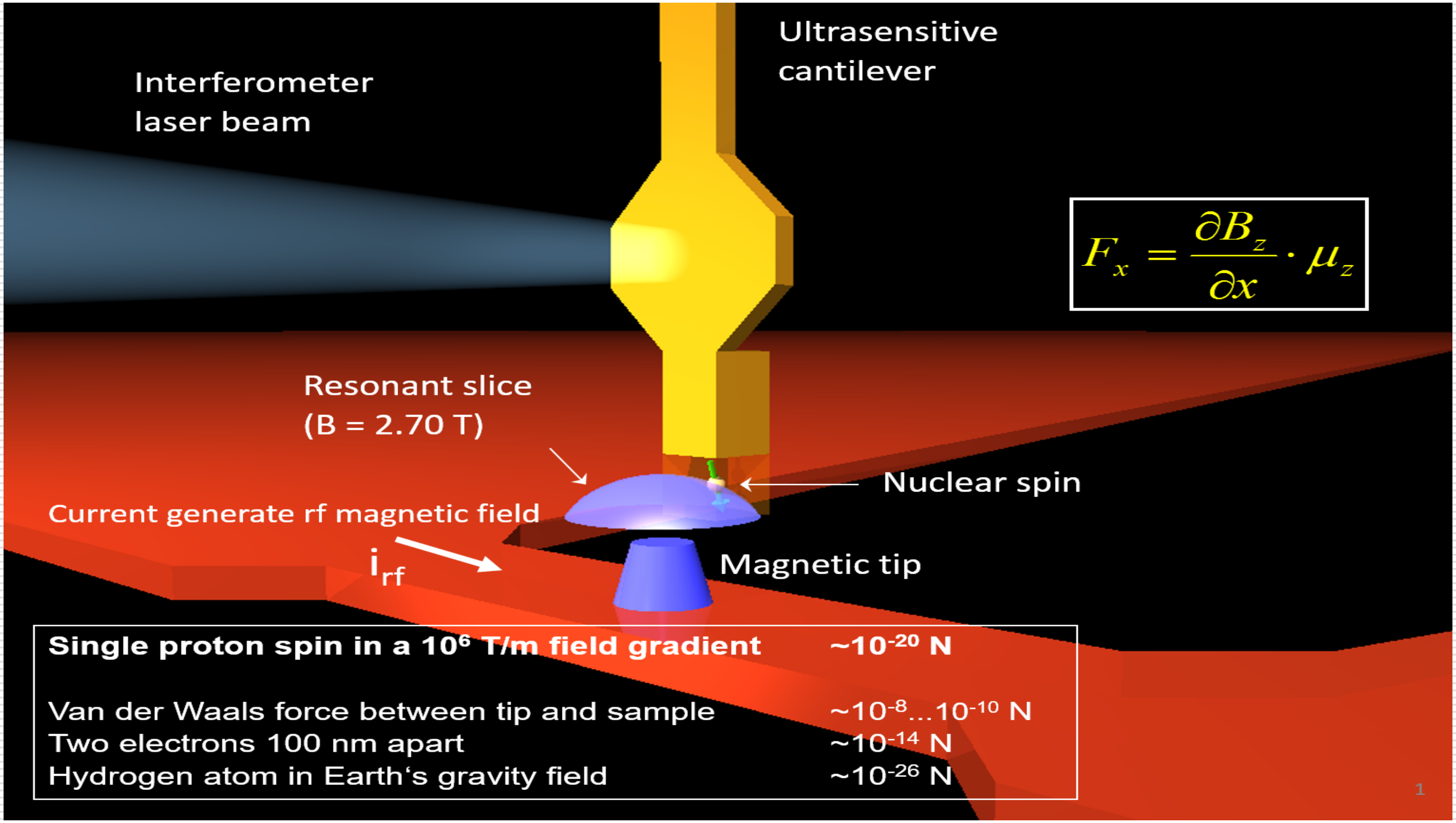
(Compatible with superconducting qubits)

Electronic:
synchronization





Force detected magnetic resonance (FMR)



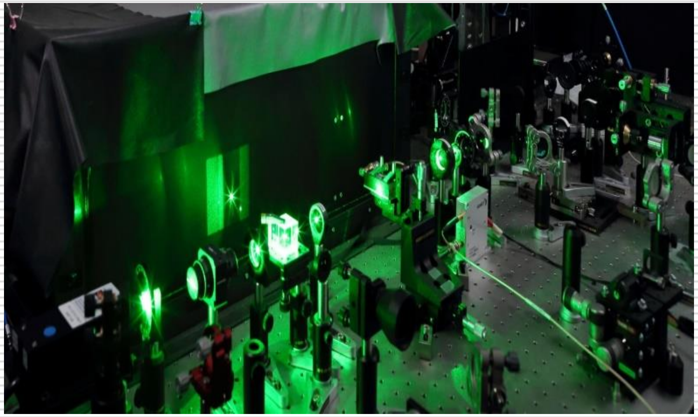
$$F_x = \frac{\partial B_z}{\partial x} \cdot \mu_z$$

Single proton spin in a 10^6 T/m field gradient	**$\sim 10^{-20}$ N**
Van der Waals force between tip and sample	$\sim 10^{-8} \ldots 10^{-10}$ N
Two electrons 100 nm apart	$\sim 10^{-14}$ N
Hydrogen atom in Earth's gravity field	$\sim 10^{-26}$ N

Experimental instruments in our lab

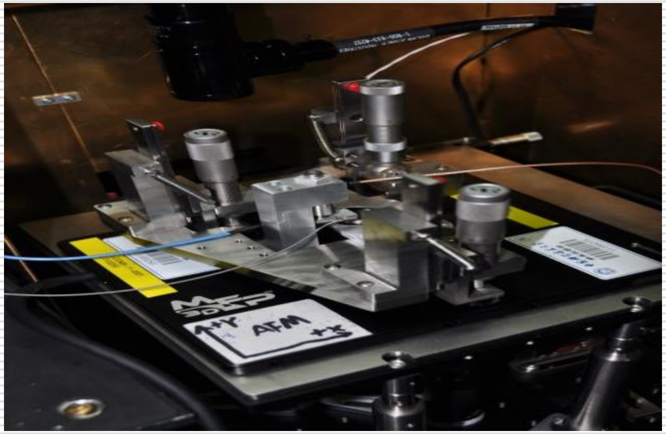
NMR

ESR



ODMR

FMR



Physical implementation of QC

DiVincenzo’s 5 criteria

- Well-defined qubits
- **Initialization to a pure state**
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DiVincenzo D.P., Fortschr. Physik, 48 (9-11), 771 – 783 (2000)
The Physical Implementation of Quantum Computation

Initialing to the pure states

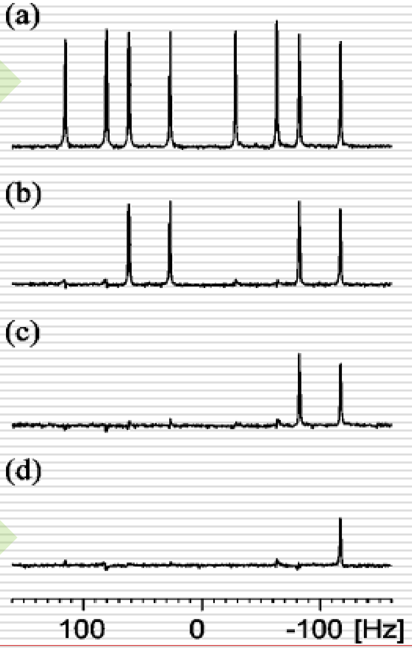
Ensemble spin case

For NMR and ESR, we prepare the Pseudo pure states (PPS).

thermal equilibrium state

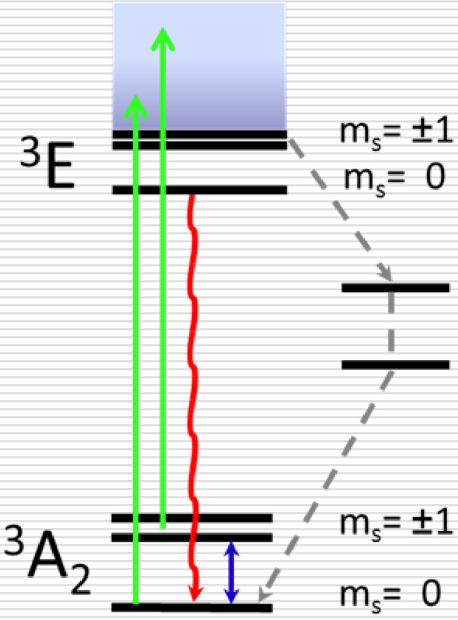
Pulse sequence for initializing

Pseudo pure states state



Single spin case

For NV center, optical pumping can prepare to the ground state $|m_s = 0>$.



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The Physical Implementation of Quantum Computation

Coherence time

A robust and fully functional quantum computer needs to have a long coherence time.

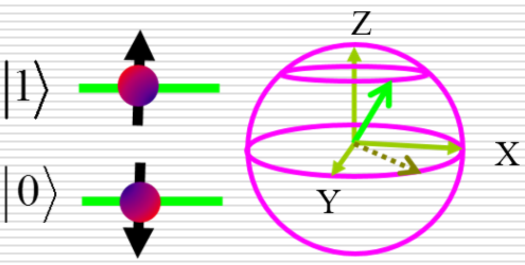
Decoherence – a major obstacle for QC

Decoherence causes errors

Main source : coupling to environment

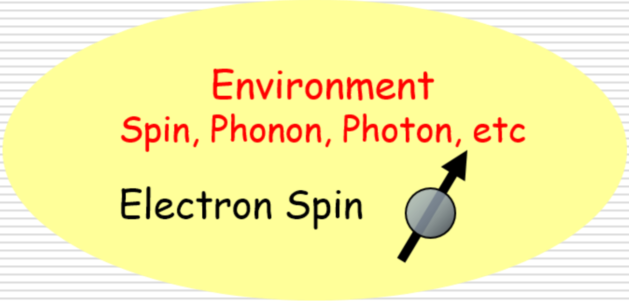
Errors are difficult to correct in Quantum Computers

Decoherence due to the environment



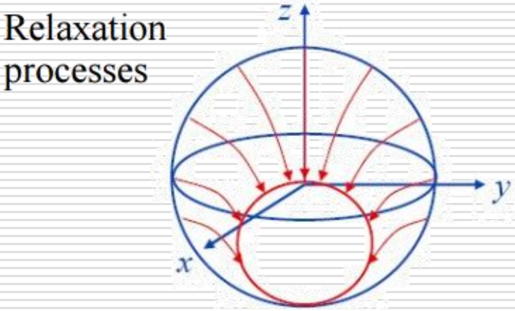
$\cos\theta|0\rangle + e^{i\phi}\sin\theta|1\rangle$

Coupling to the environment

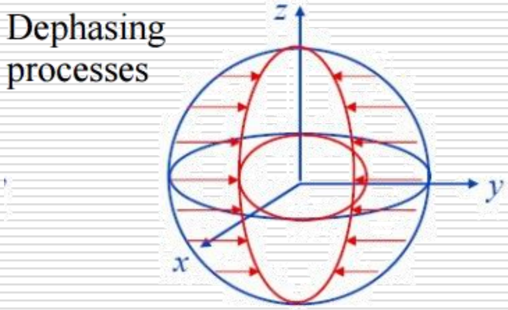


<u>Energy relaxation (T_1):</u>
Spin system will 'relax' towards the ground state given enough time.

<u>Dephasing (T_2):</u>
The phase information becomes spread out / lost.



Usually $T_2 \ll T_1$



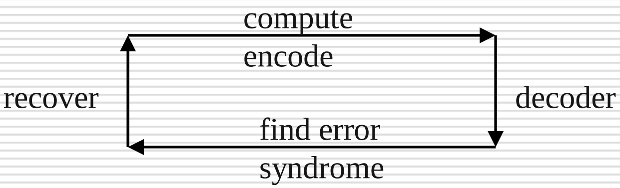
Graphic from http://qt.tn.tudelft.nl/~lieven/qip2007/QIP3_divincenzo_criteria.pdf

How to protect the quantum state

- Quantum error correcting codes

works best for errors uncorrelated in space and time.

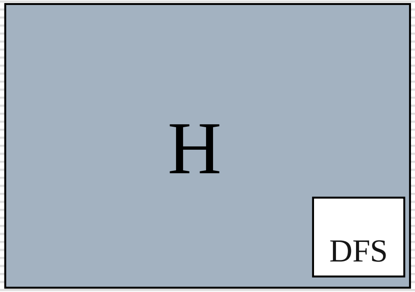
P. W. Shor, Phys. Rev. A 52, R2493 (1995
A.M. Steane, Phys. Rev. Lett. 77, 793 (1996).
E. Knill and R. Laflamme, Phys. Rev. A 55, 900 (1997)



- Decoherence-free subspaces

assumes symmetry in H (strongly correlated errors).

L. M. Duan and G. C. Guo, Phys. Rev. Lett. 79, 1953 (1997).
D. A. Lidar, I. L. Chuang, and K. B. Whaley, Phys. Rev. Lett. 81, 2594 (1998).

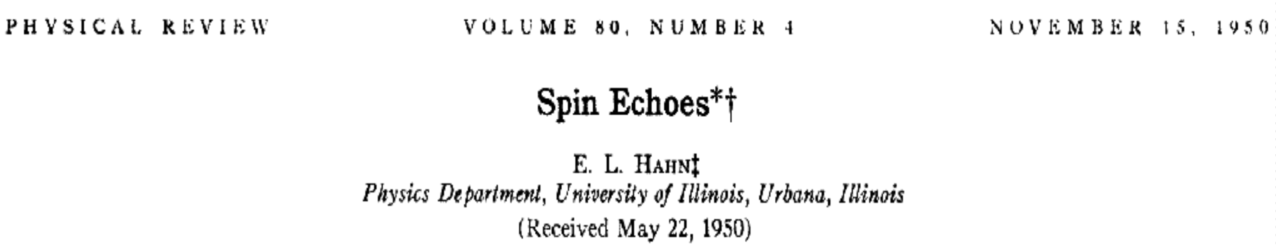


- Dynamical decoupling (DD)

very rapid, strong pulses

L. Viola and S. Lloyd, Phys. Rev. A 58, 2733 (1998).
M. Ban, J. Mod. Opt. 45, 2315 (1998).

Dynamical Decoupling



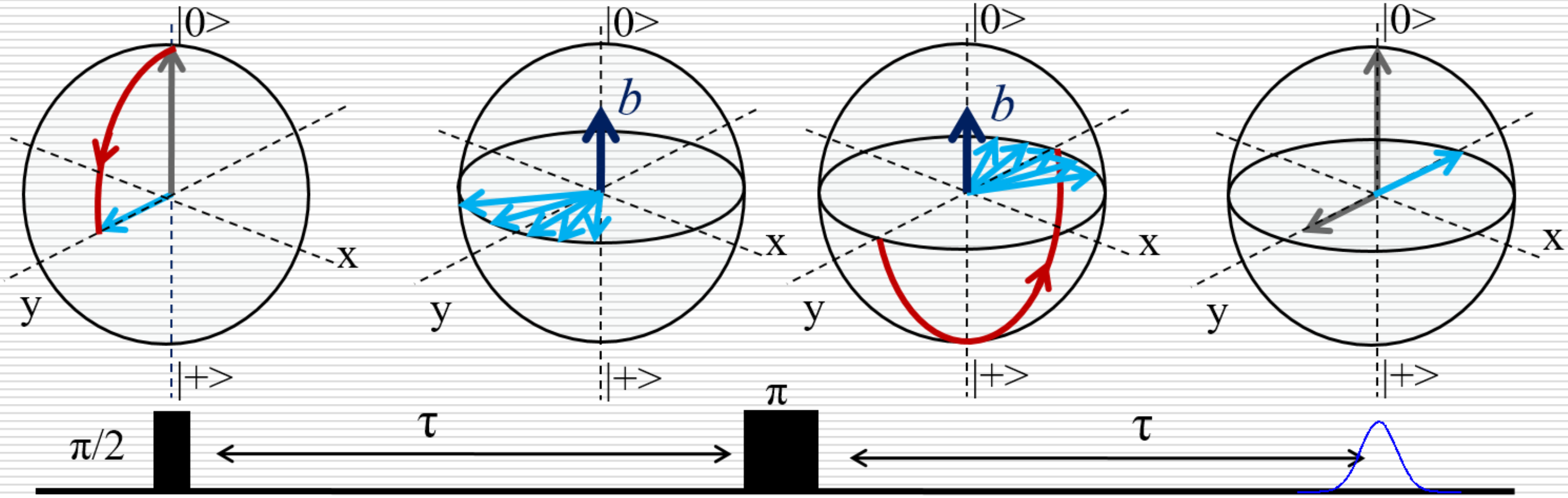
PHYSICAL REVIEW VOLUME 80, NUMBER 4 NOVEMBER 15, 1950

Spin Echoes*†

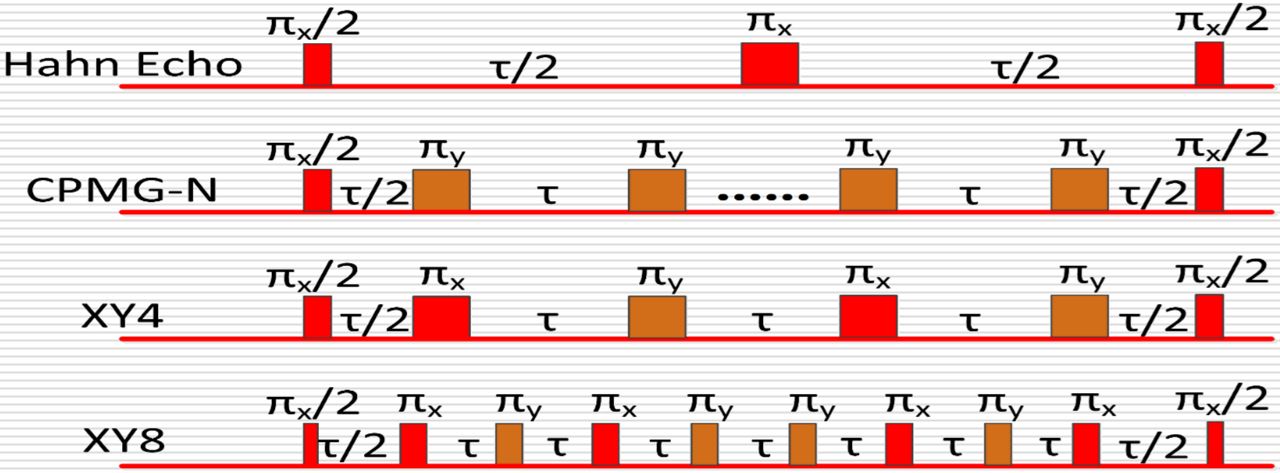
E. L. HAHN‡
Physics Department, University of Illinois, Urbana, Illinois

(Received May 22, 1950)

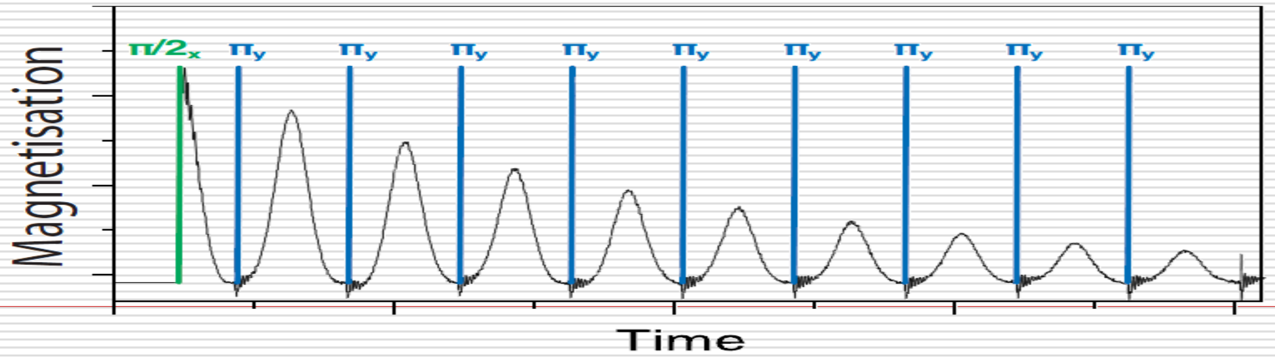
$|0\rangle + |1\rangle$ $|0\rangle + e^{ib\tau}|1\rangle$ $|0\rangle + e^{-ib\tau}|1\rangle$ $|0\rangle + e^{-ib\tau + ib\tau}|1\rangle$



Multi-Pulse Dynamical Decoupling



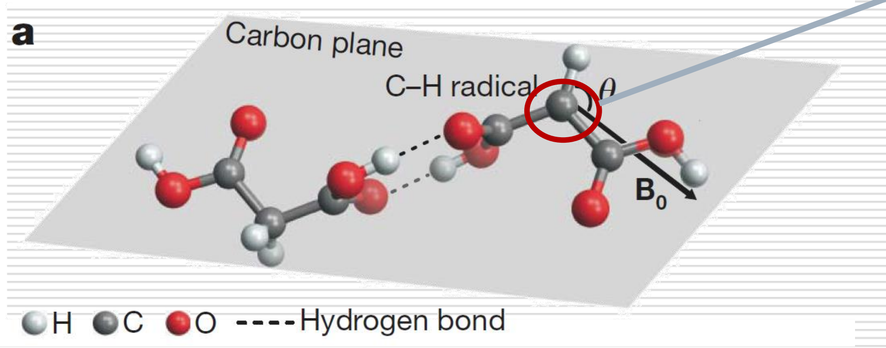
Example: CPMG on N@C60

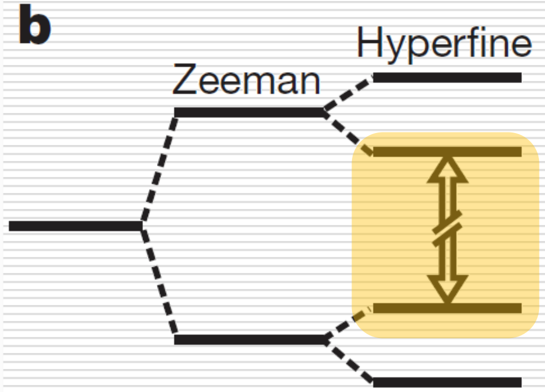


Keep a qubit alive by dynamical decoupling

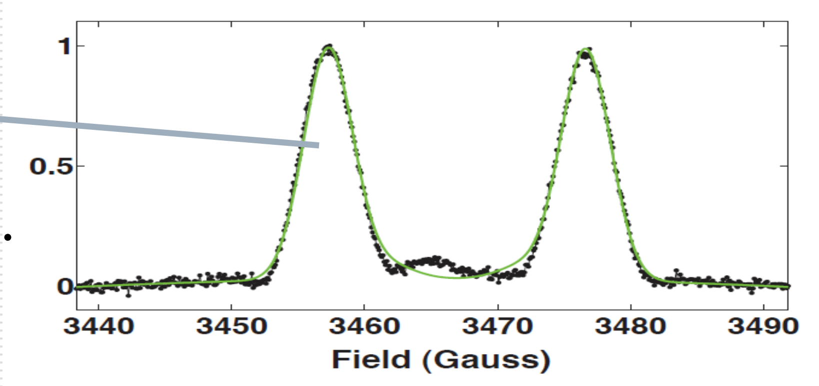
Sample: irradiated malonic acid

Two energy levels of electron spin are encoded as a qubit





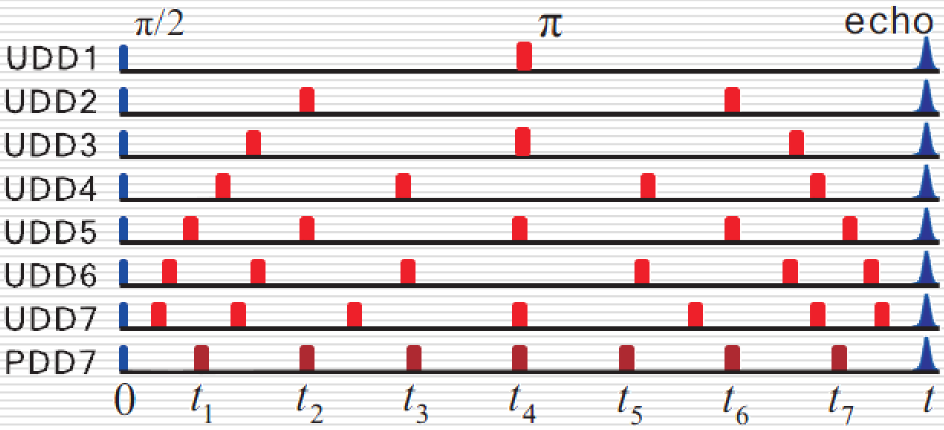
Broadening of the linewidth indicates that the electronic qubit interacts with the nuclear spin bath. Related coherence time: 40 ns

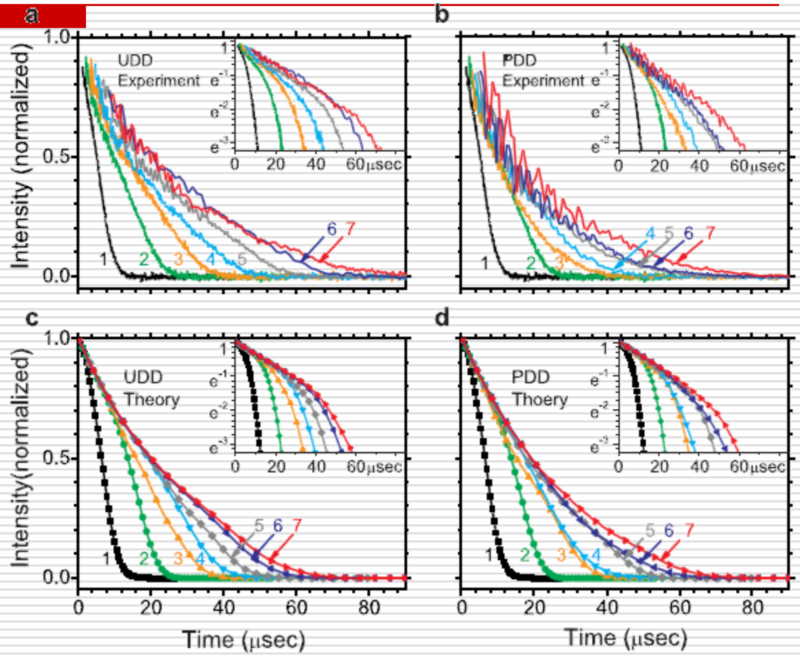


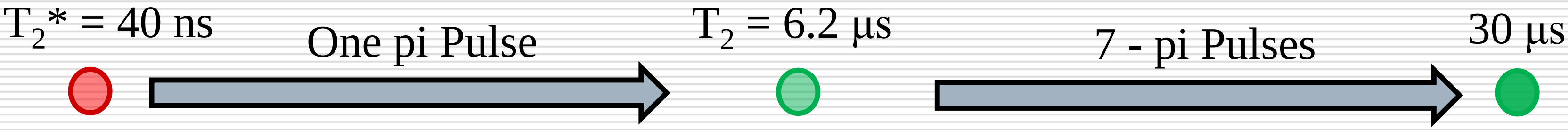
J. Du et al., Nature 461, 1265 (2009)

Keep a qubit alive by dynamical decoupling

Apply DD on the electronic qubit






$T_2^* = 40$ ns

One pi Pulse

$T_2 = 6.2$ μs

7 - pi Pulses

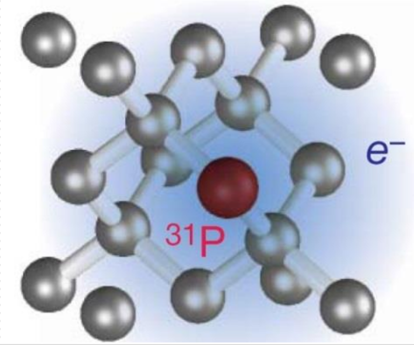
30 μs

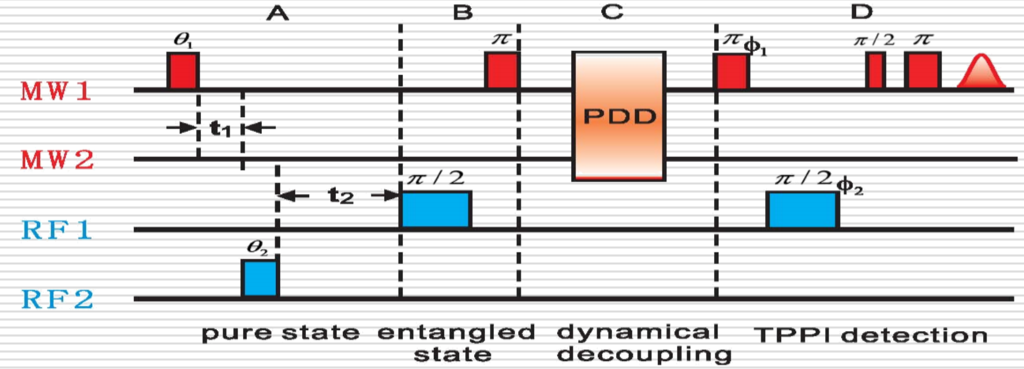
An improvement of near three orders of magnitude on the spin coherence time was observed in the experiment.

J. Du et al., Nature 461, 1265 (2009)

Keep entanglement alive

Si:P





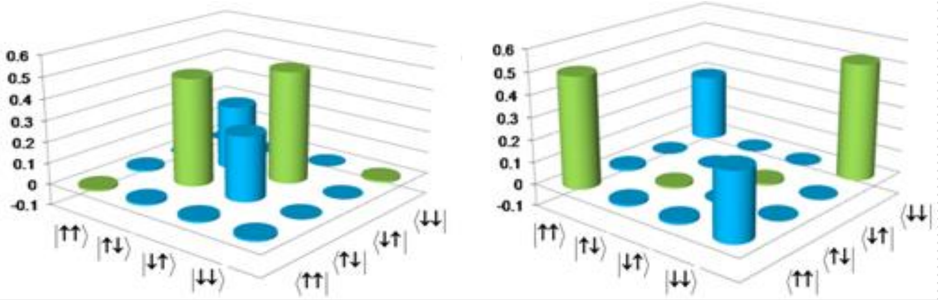
Life time of entanglement

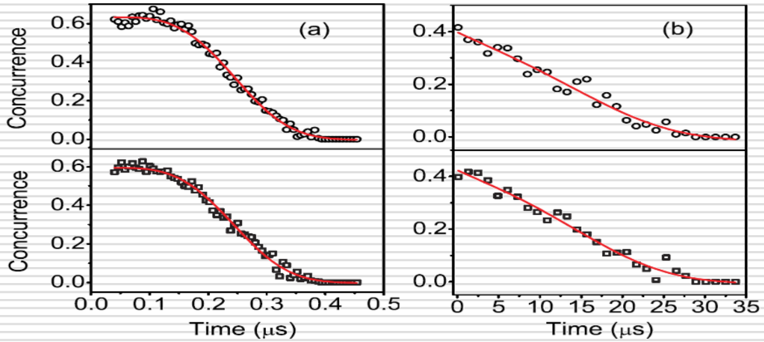
With DD: 30 μs

No DD: 0.4 μs

Preparation of entanglement states

Protection of entanglement





Y. Wang et al., Phys. Rev. Lett. 106, 040501 (2011)

Physical implementation of QC

DiVincenzo's 5 criteria

- Well-defined qubits
- Initialization to a pure state
- Long coherence times
- **Universal set of quantum gates**
- Qubit-specific measurement

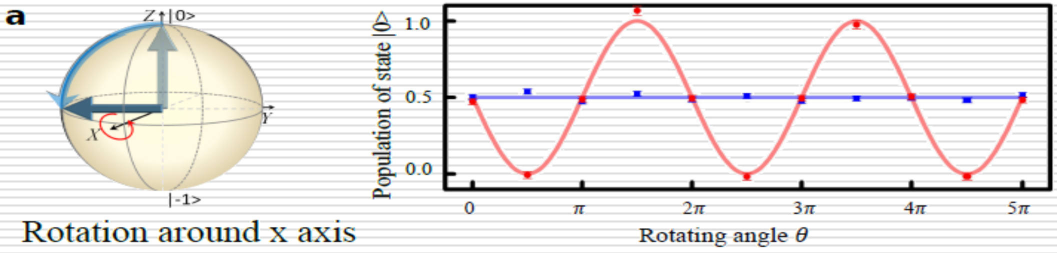
DiVincenzo D.P., Fortschr. Physik, 48 (9-11), 771 – 783 (2000)
The Physical Implementation of Quantum Computation

Universal set of quantum gates

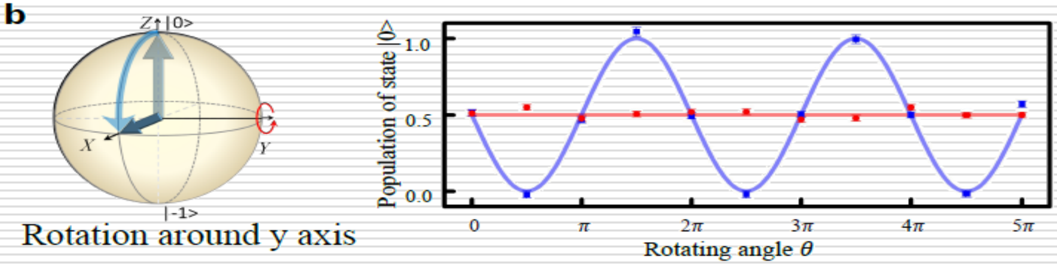
☐ Single-qubit gates

Rotations around any two non-parallel rotation axis.

$$R_X(\theta) = e^{-i\theta/2 \cdot X}$$
$$R_Y(\theta) = e^{-i\theta/2 \cdot Y}$$



Rotation around x axis



Rotation around y axis

☐ Two-qubit gates

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \qquad \mathrm{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \qquad \mathrm{Cphase} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\alpha} & 0 \\ 0 & 0 & 0 & e^{i\alpha} \end{pmatrix}$$

CNOTs and unitary single Qbit operations form an universal set of QC

Characterize quantum gates

- ☐ Quantum Process Tomography (QPT)

$$\rho_f = \sum_k A_k \rho_i A_k^\dagger = \sum_{kl} \chi_{kl} P_k \rho_i P_l$$

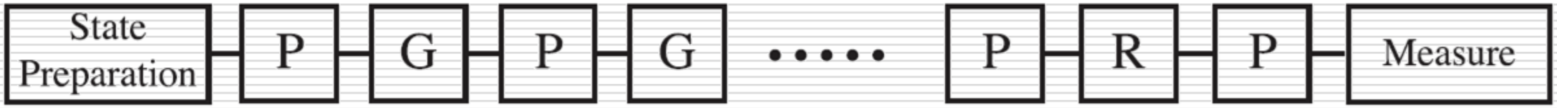
For single-qubit,

Figure from http://aspuru.chem.harvard.edu/excitonics/

Measuring fidelities of quantum gates

- Randomized benchmarking

single-qubit case

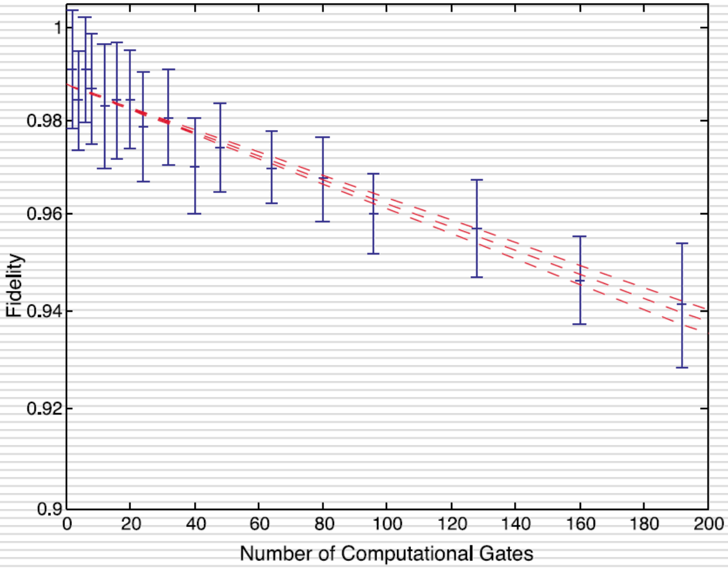


State Preparation P G P G ····· P R P Measure

P Pauli Gates: π gate around the $\pm x$, $\pm y$, or $\pm z$ axes and I identity gate

G Clifford Gates: $\pi/2$ gate around the $\pm x$, $\pm y$, or $\pm z$ axes

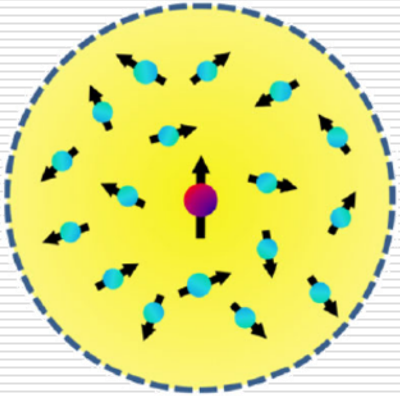
R Recovery Gates: a final Clifford gate chosen to make the final state $|0\rangle$



C. A. Ryan et al., NJP 11, 013034 (2009)

Quantum gates under noises

single-qubit case



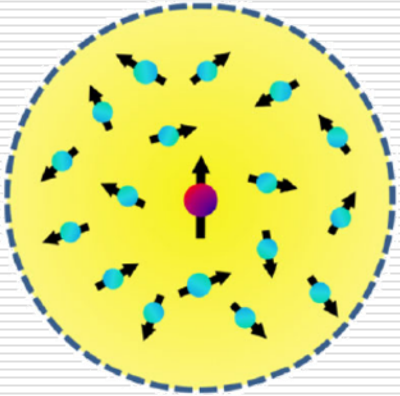
$$H = \boxed{\delta_0}\, Sz + (1 + \boxed{\delta_1})\, \omega_1\, Sx$$

Dephasing effect

Noise from the control field

- ➢ How to suppress the dephasing effect ?
- ➢ How to suppress the noise from the control field ?
- ➢ How to suppress both simultaneously ?

Challenge of Protecting Quantum Gates



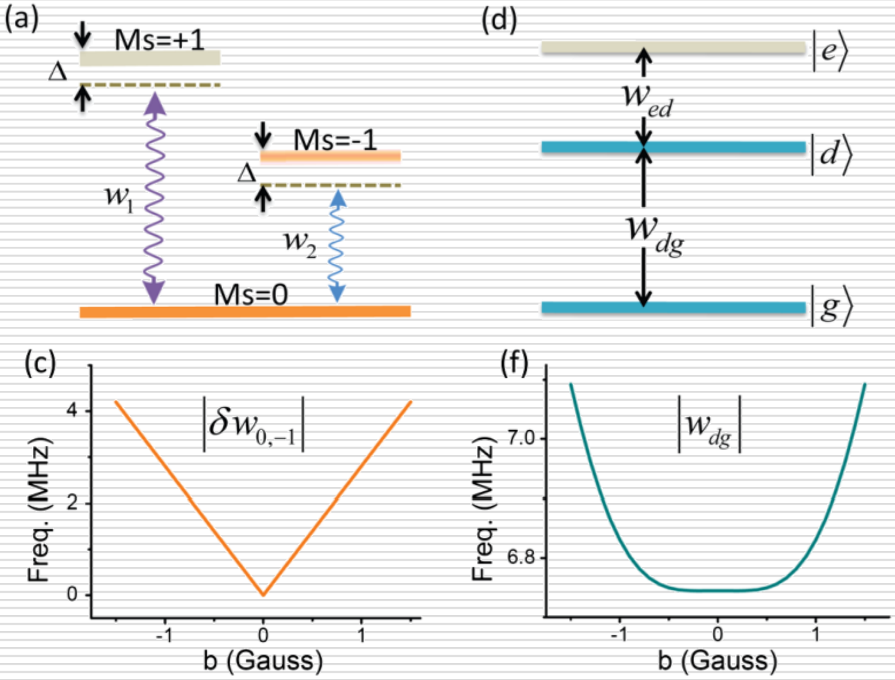
$$H = \boxed{\delta_0} Sz + (1 + \boxed{\delta_1}) \omega_1 Sx$$

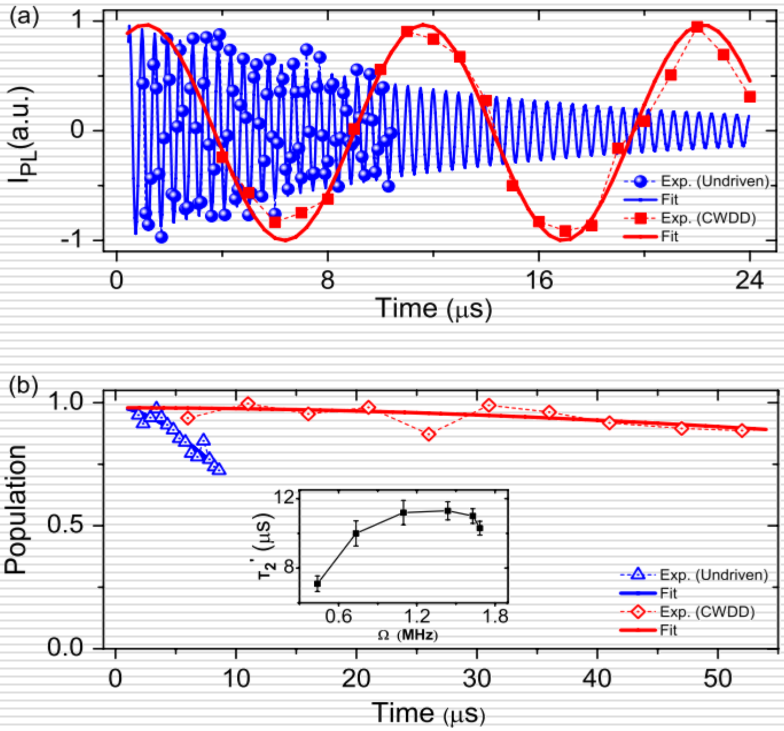
Dephasing effect

Noise from the control field

- ➢ How to suppress the dephasing effect ?
- ➢ How to suppress the noise from the control field ?
- ➢ How to suppress both simultaneously ?

Protect gates by continuous dynamical decoupling





Sensitive

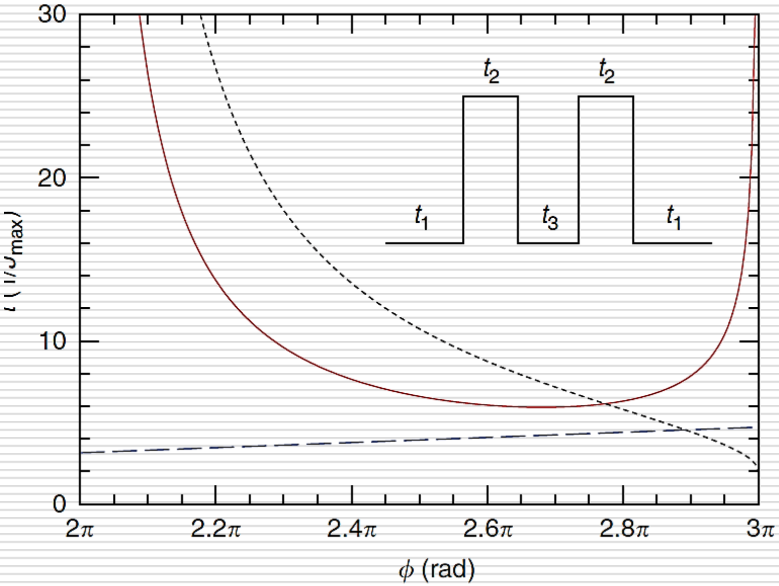
Robust

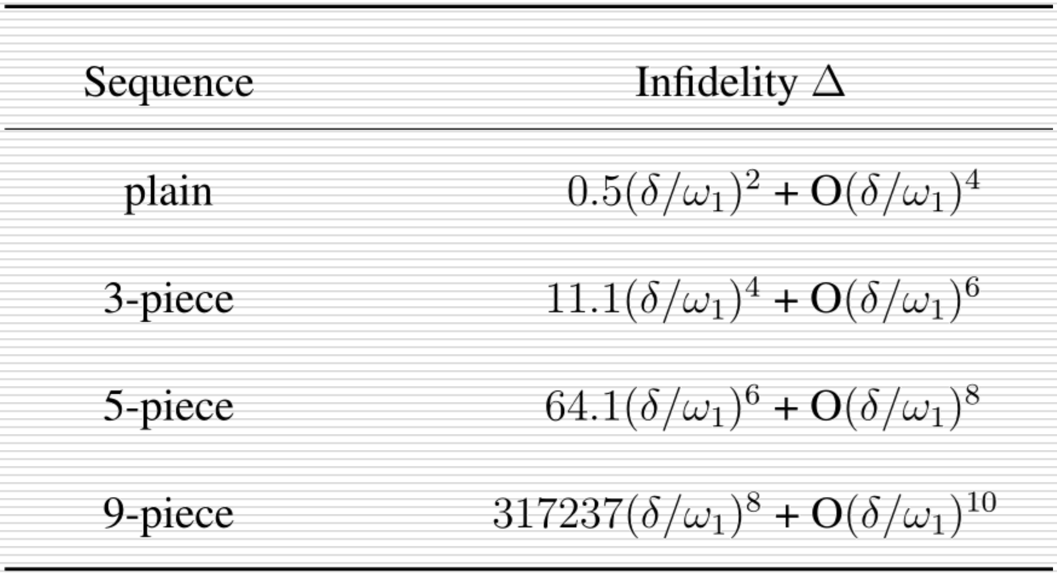
Blue : without CWDD
Red : with CWDD

X. Xu et al., Phys. Rev. Lett. 109, 070502 (2012)

Dynamically corrected gates

$$H = \delta\, S_z + \omega_1\, S_x$$





Sequence	Infidelity Δ
plain	$0.5(\delta/\omega_1)^2 + O(\delta/\omega_1)^4$
3-piece	$11.1(\delta/\omega_1)^4 + O(\delta/\omega_1)^6$
5-piece	$64.1(\delta/\omega_1)^6 + O(\delta/\omega_1)^8$
9-piece	$317237(\delta/\omega_1)^8 + O(\delta/\omega_1)^{10}$

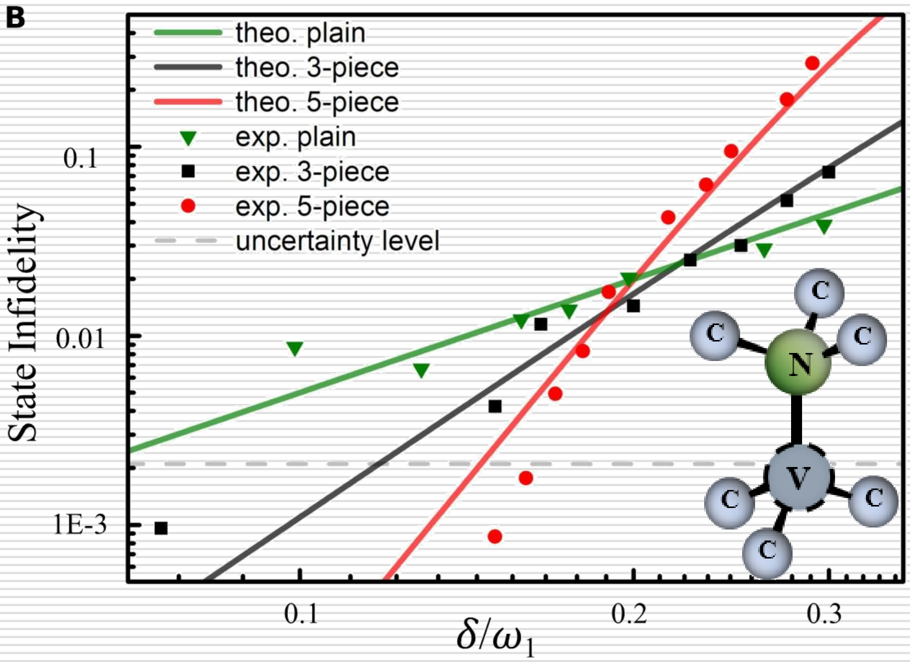
We adopted this proposal to overcome the deterioration of quantum gates by the fluctuation of the static magnetic field.

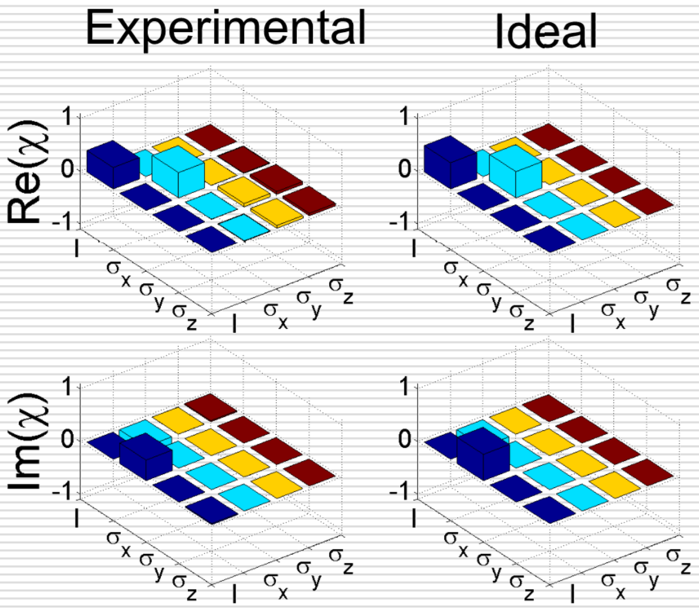
Xin Wang et al., Nat. Commun. 3, 997 (2012)

Experimental dynamically corrected gates

Suppressing the noise up to 6 order

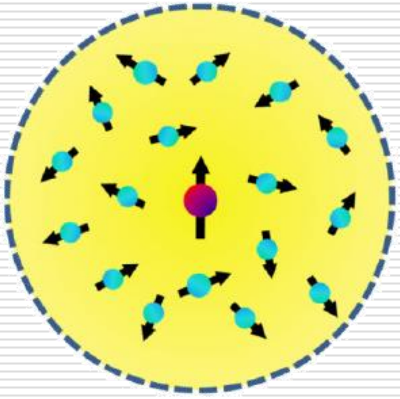
Fidelity of the gate reaches 0.996





X. Rong et al., Phys. Rev. Lett. 112, 050503 (2014)

Challenge of protecting quantum gates



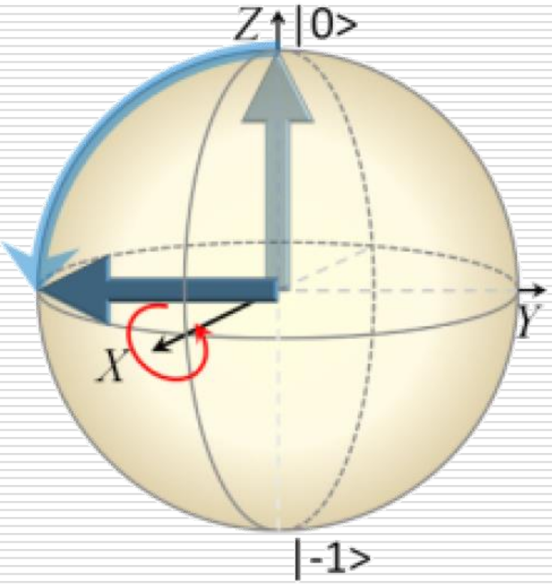
$$H = \delta_0\ Sz + (1 + \delta_1)\ \omega_1\ Sx$$

Dephasing effect

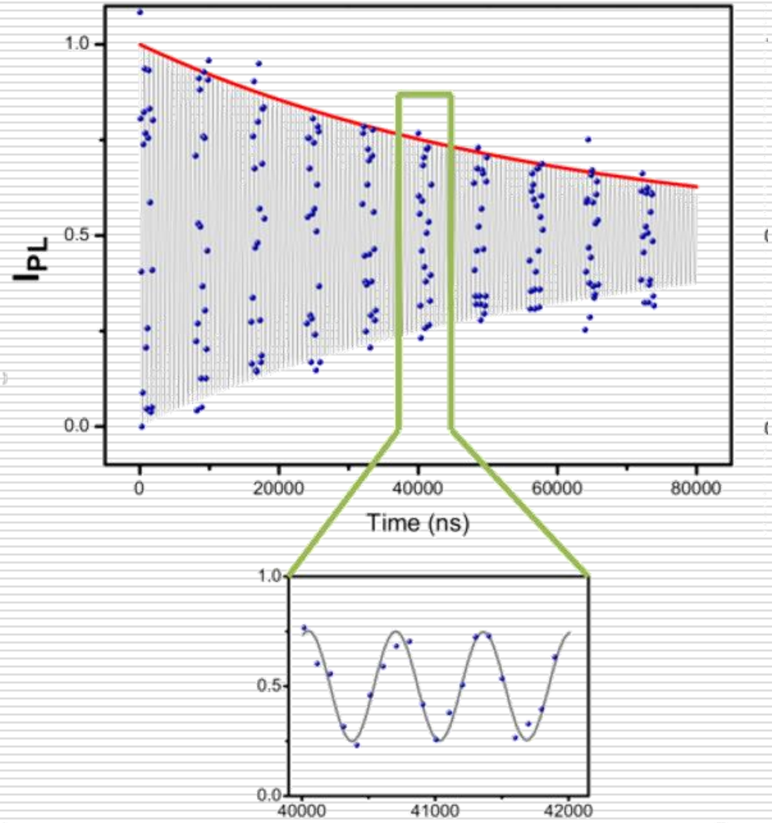
Noise from the control field

- ➢ How to suppress the dephasing effect ?
- ➢ How to suppress the noise from the control field ?
- ➢ How to suppress both simultaneously ?

Noise from the control field



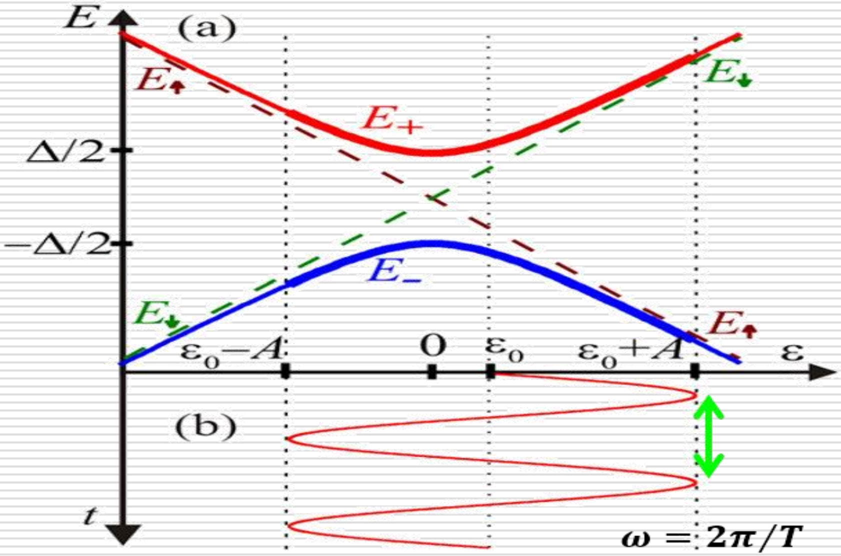
T2’=17 us

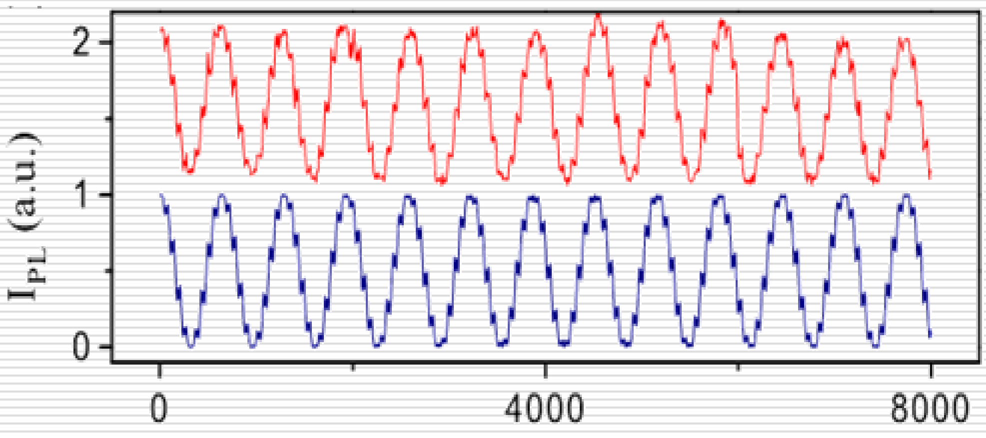


$$H = (1 + \delta)\, \omega_1\, S_x$$

J. Zhou et al., Phys. Rev. Lett. 112, 010503 (2014)

Theoretical proposal





υ= 3.12 MHz/ns

Hamiltonian

$$H_{LZ} = (1+\delta)\Delta S_x + (\varepsilon_0 + A\cos\omega t)S_z$$

Energy gap Δ; Amplitude of the freq. sweeping A

After carefully setting these parameters, multiple LZ transitions can produce period Rabi oscillations.

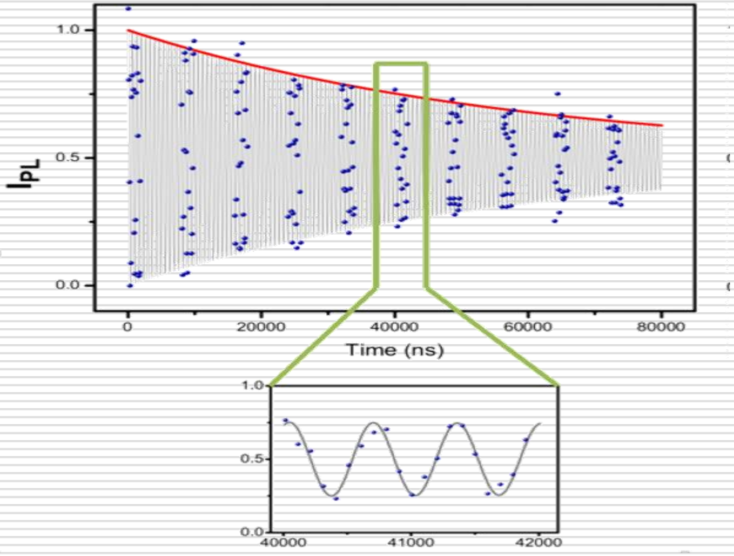
J. Zhou et al., Phys. Rev. Lett. 112, 010503 (2014)

Suppressing the noise from the control Field

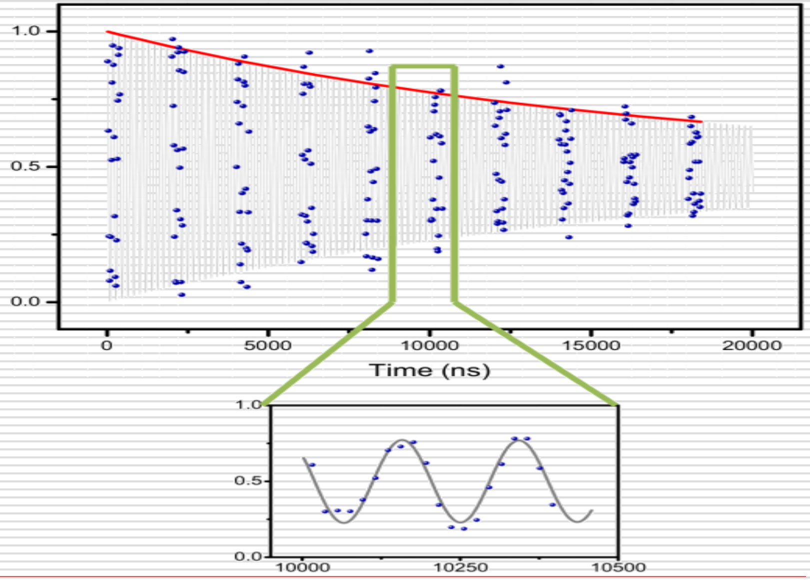
Theoretical calculations shows that $T'_{2,LZRO} = T'_2/|J_n(A/\omega)|$

where $n = \varepsilon_0/\omega$, since $|J_n(A/\omega)| < 1$ LZRO's T_2' can be greatly prolonged

T2'=17 us

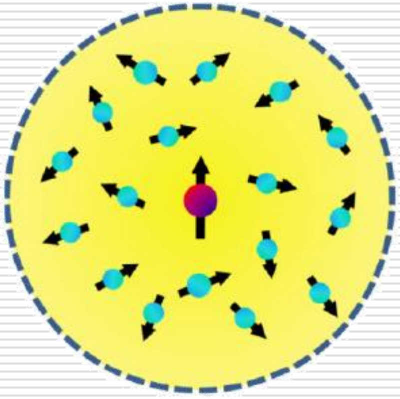


$T'_{2,LZRO} = 58\ us$



J. Zhou et al., Phys. Rev. Lett. 112, 010503 (2014)

Challenge of protecting quantum gates



$$H = \boxed{\delta_0} Sz + (1 + \boxed{\delta_1}) \omega_1 Sx$$

Dephasing effect

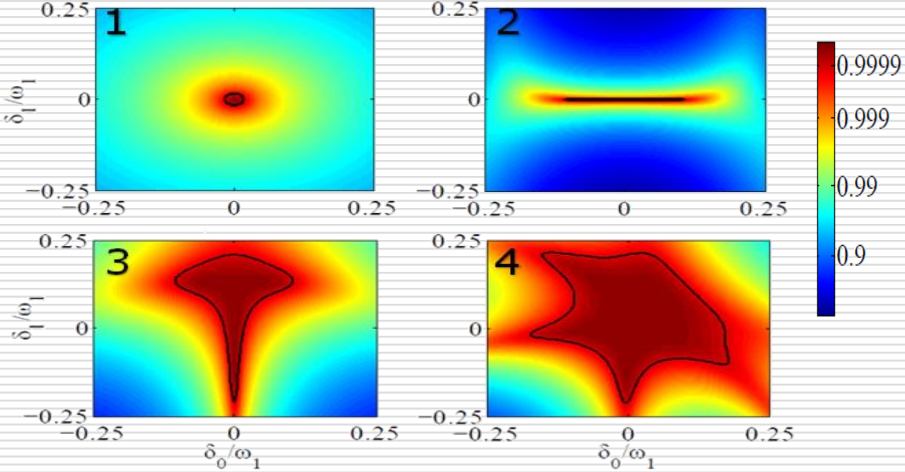
Noise from the control field

- ➢ How to suppress the dephasing effect ?
- ➢ How to suppress the noise from the control field ?
- ➢ How to suppress both simultaneously ?

Composite pulse for high-fidelity gates

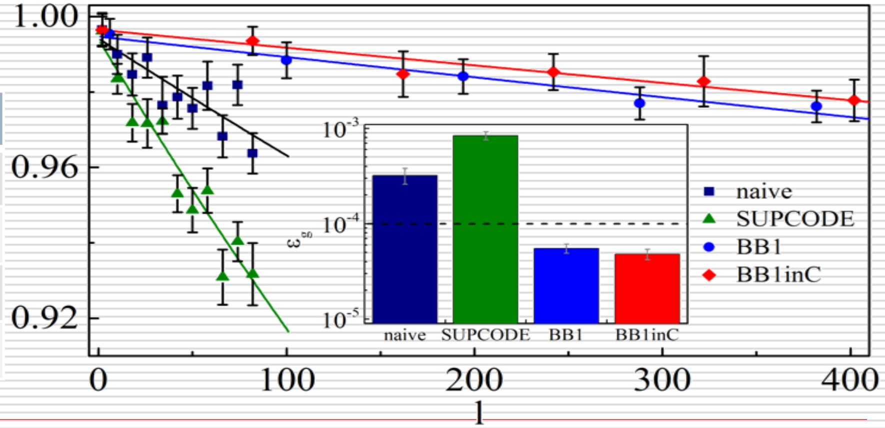
$$H = \delta_0\, Sz + (1 + \delta_1)\, \omega_1\, Sx$$

scheme	suppressing	
	δ_0	δ_1
1. rectangle	☹	☹
2. SUPCODE	☺	☹
3. BB1	😐	☺
4. BB1inC	☺	☺



Exp. results

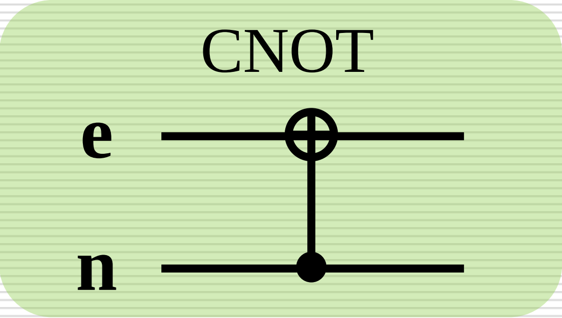
scheme	Fidelity
1. rectangle	0.99968
2. SUPCODE	0.99916
3. BB1	0.99994
4. BB1inC	0.99995



X. Rong et al., arXiv:1506.08627 (2015)

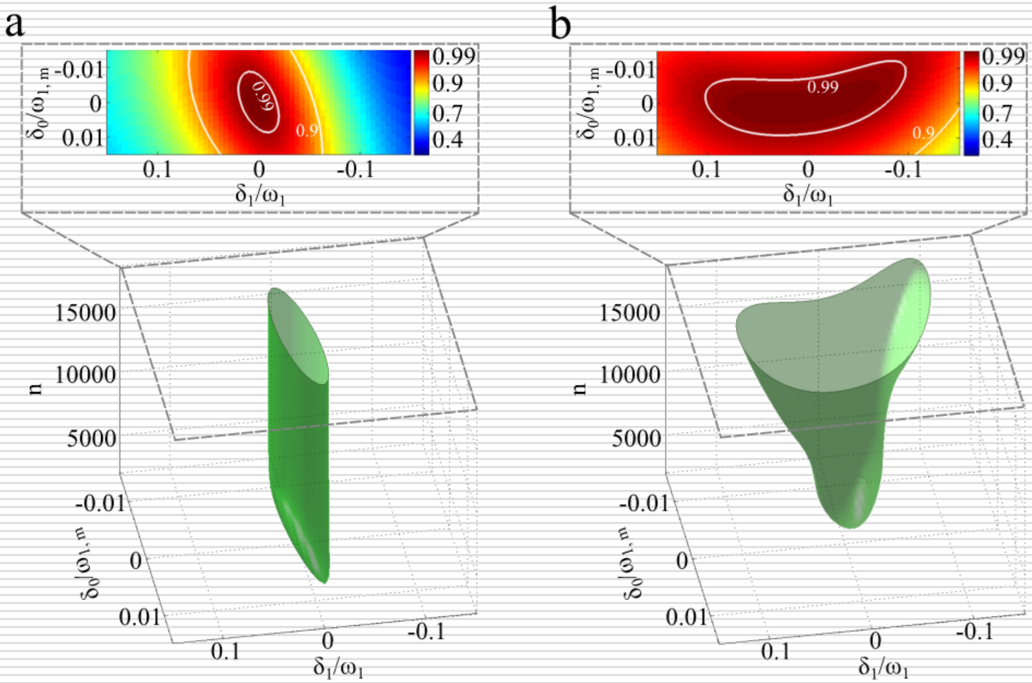
Protecting two-qubit gates

Quantum optimal control can help us to design pulse sequence, which are robust against noises in multi-qubit cases.



Original quantum optimal control method [1]

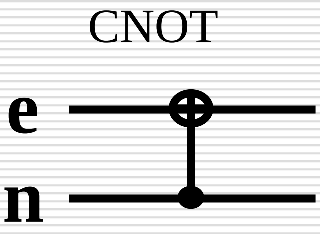
Modified quantum optimal control method [2]



[1] N. Khaneja et al., J. Magn. Reson. 172, 296 (2005)

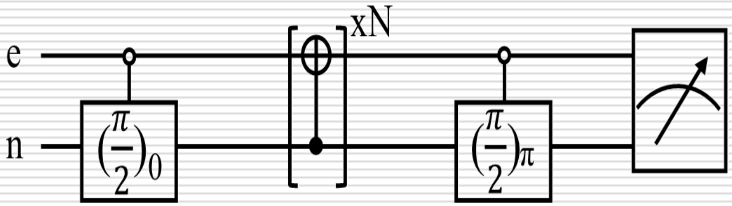
[2] X. Rong et al., Nat. Commun. 6, 8748 (2015)

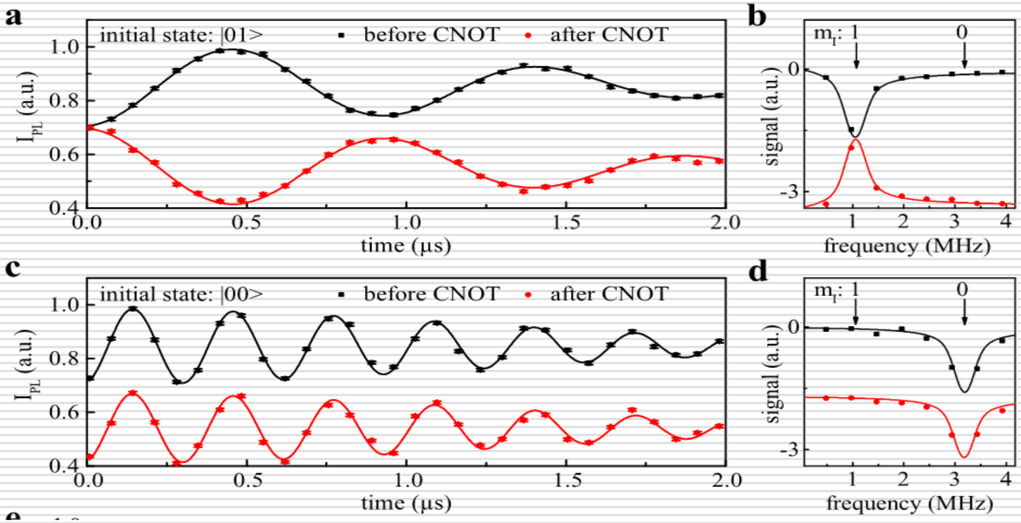
Qualify the performance of CNOT



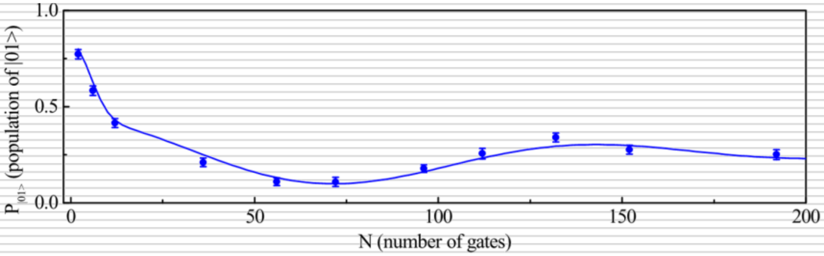
Before CNOT		After CNOT	
e	n	e	n
|0>	|1>	|1>	|1>
|0>	|0>	|0>	|0>

Measuring the fidelity of CNOT





Experimental results:



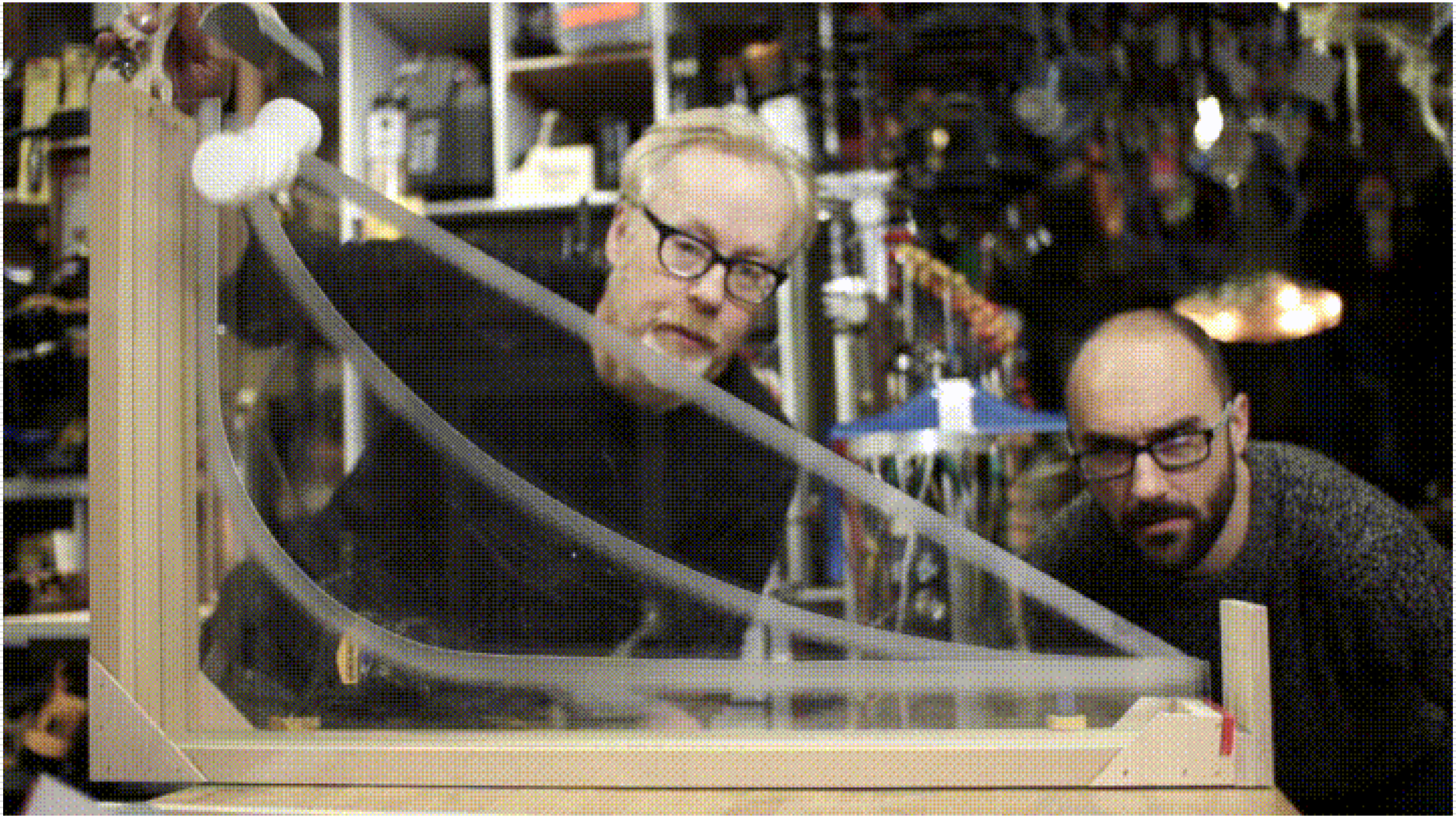
Theoretical fidelity	Experimental fidelity
0.9927	0.9920(1)

X. Rong et al., Nat. Commun. 6, 8748 (2015)

Two questions

- Since control can be performed with high fidelities, can we operate the quantum gates as fast as possible (in a time-optimal way) ?

- If the gate is carried out in a time-optimal way, does the high fidelity still hold?

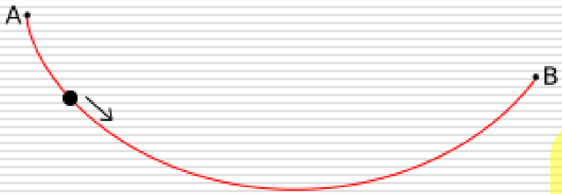


gif from https://giphy.com/

Experimental time optimal quantum control

- ☐ Can we drive the quantum system as fast as possible?

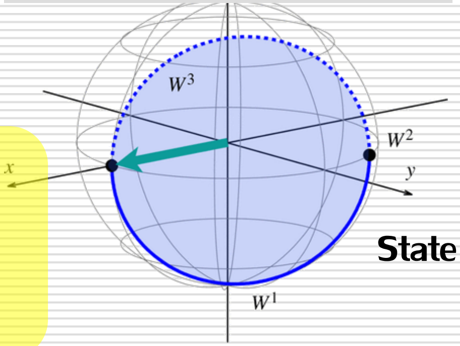
Classical version



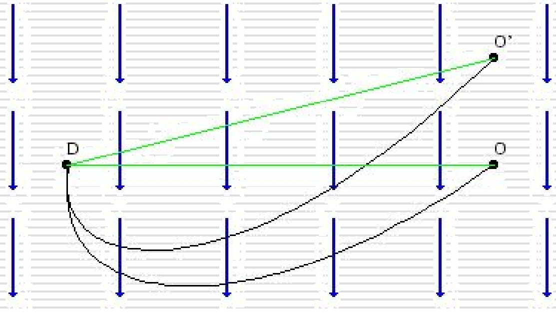
Brachistochrone

shortest time

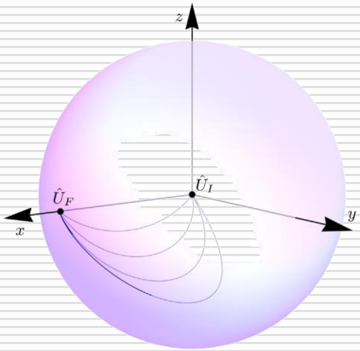
Quantum version



State to state



Zermelo Navigation



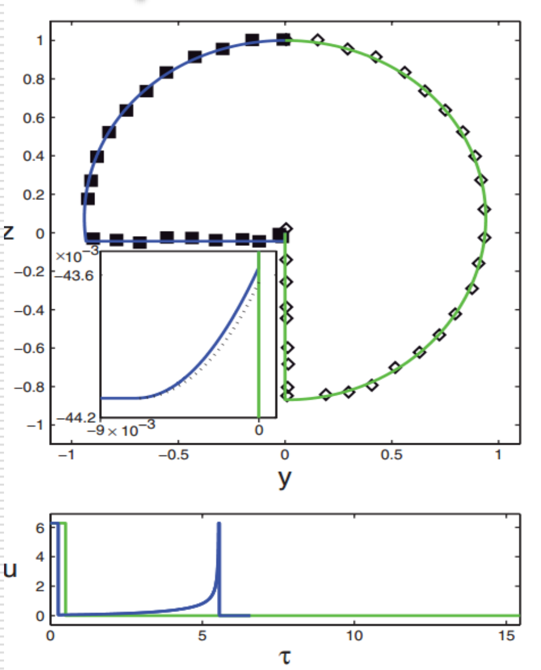
U to U

Previous experimental work

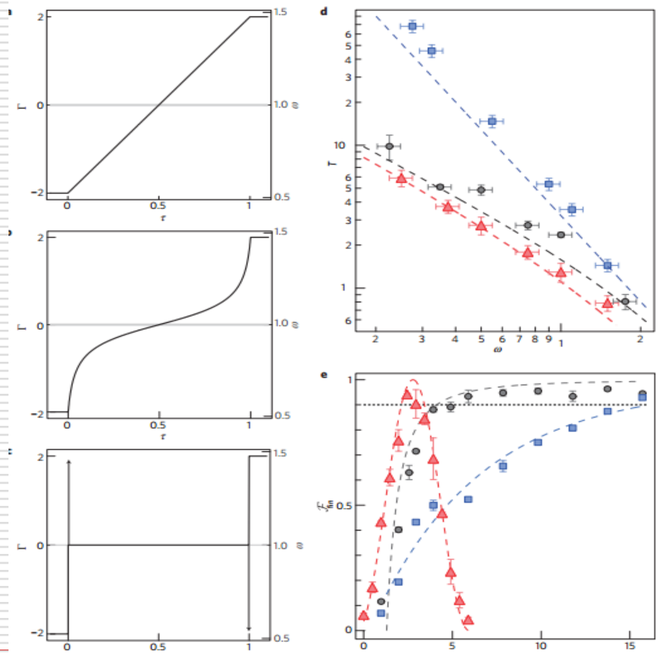
single qubit case

state to state

unitary operations



PRL 104, 083001 (2010)



Nature Phys 8, 147-152 (2012)

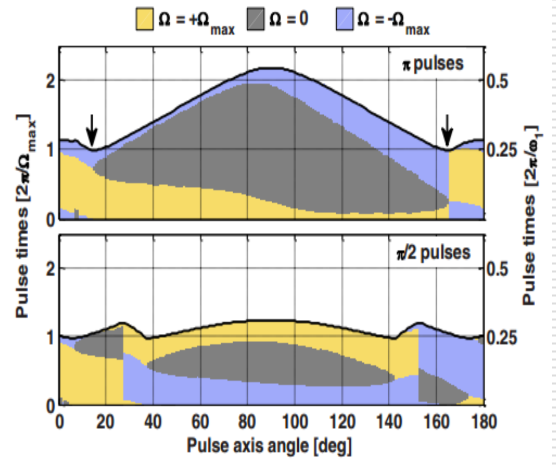
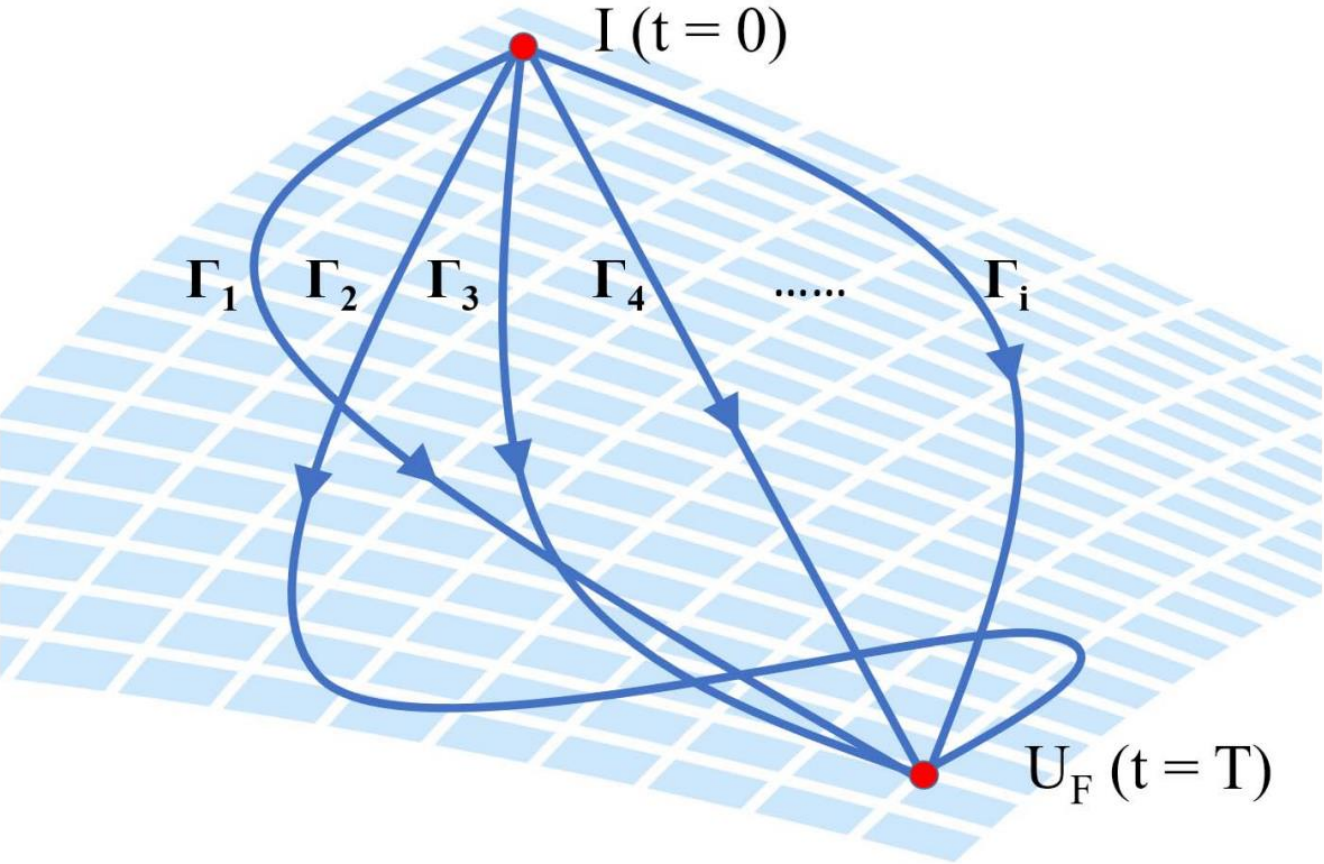
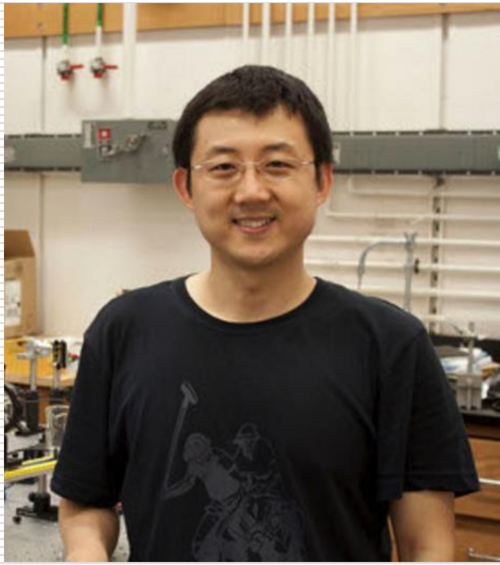


FIG. 1. (Color online) Time-optimal pulse sequences for generating $\pi/2$ and π rotations (top and bottom panels, respectively), for $\Omega_{max} = 4\omega_1$. Colors represent different types of pulses: positive/negative bangs and drift. Black arrows mark the globally optimal π rotations, corresponding to pure bang-bang controls.

PRB 89, 245311 (2014)

Time-optimal control beyond one-qubit



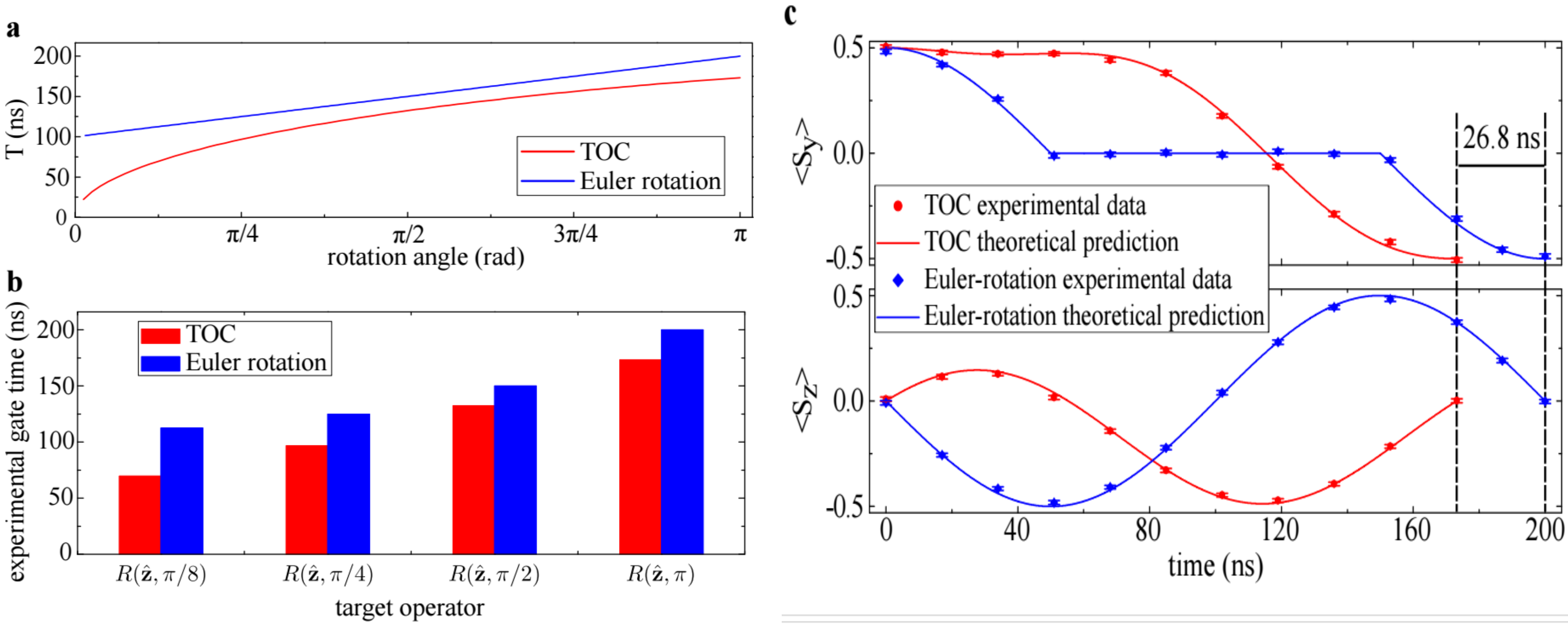


One can find solutions for time-optimal control (TOC) in multi-qubit cases.

X. Wang, et al., Phys. Rev. Lett. 114, 170501 (2015)

One-qubit case: TOC v.s. Euler Rotation

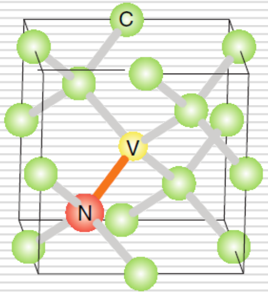
- Target operation: R(z,θ)
- Control field is restricted in x / y axis with a finite strength (5 MHz).

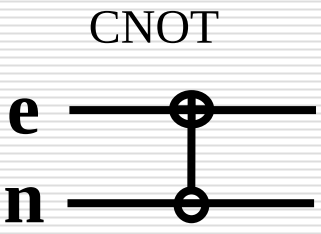


J. Geng et al., Phys. Rev. Lett. 117, 170501(2016)

Two-qubit case: CNOT gate

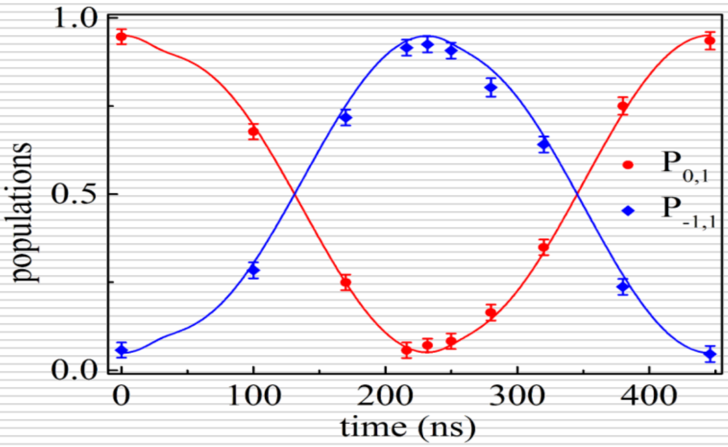
Quantum system: NV center



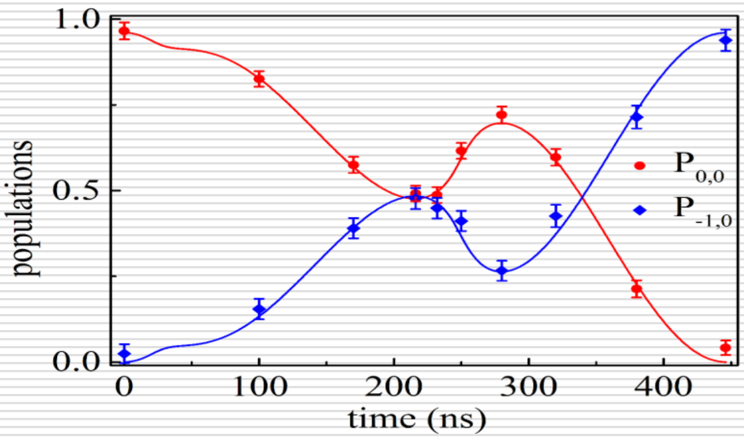


Before CNOT		After CNOT	
e	n	e	n
|0>	|0>	|-1>	|0>
|0>	|1>	|0>	|1>

Electron spin unchanged, when $|1>_n$



Electron spin is flipped, when $|0>_n$



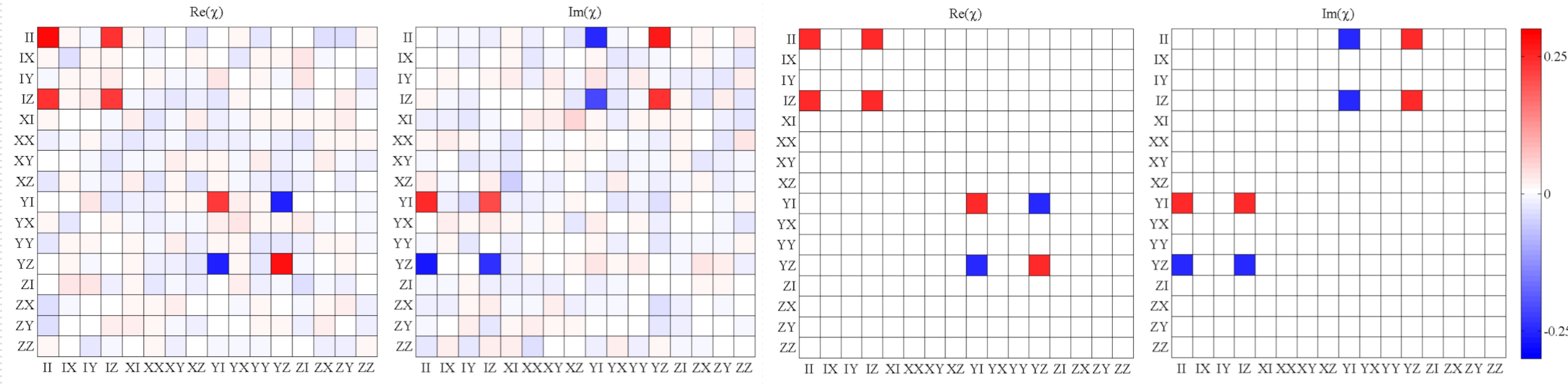
J. Geng et al., Phys. Rev. Lett. 117, 170501(2016)

Two-qubit case: CNOT gate

☐ Fidelity : 0.99(1)

Experiment result

Ideal case



	Max Strength of the control field	Fidelity	Gate time
Ref [1]	20.0 MHz	0.9920(1)	696 ns
This work [2]	2.5 MHz	0.99(1)	446 ns

---

[1] X. Rong et al., Nature Communications 6, 8748 (2015)

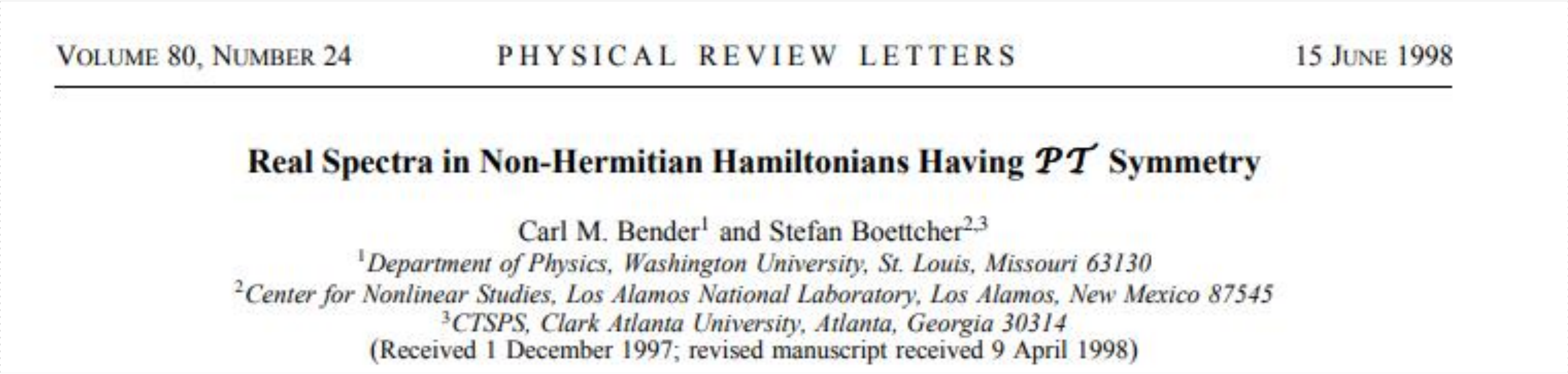
[2] J. Geng et al., Phys. Rev. Lett. 117, 170501(2016)

Quantum control beyond Hermitian Hamiltonian

- The previous results are based on Hermitian Hamiltonian.
- Now we will show how to realize quantum control with non-Hermitian Hamiltonian.
- An example:

$$H_s = \begin{bmatrix} ir & 1 \\ 1 & -ir \end{bmatrix}$$

- Hs is a parity-time symmetric Hamiltonian rather than a Hermitian one.



VOLUME 80, NUMBER 24 PHYSICAL REVIEW LETTERS 15 JUNE 1998

Real Spectra in Non-Hermitian Hamiltonians Having $\mathcal{PT}$ Symmetry

Carl M. Bender[1] and Stefan Boettcher[2,3]
[1]*Department of Physics, Washington University, St. Louis, Missouri 63130*
[2]*Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[3]*CTSPS, Clark Atlanta University, Atlanta, Georgia 30314*

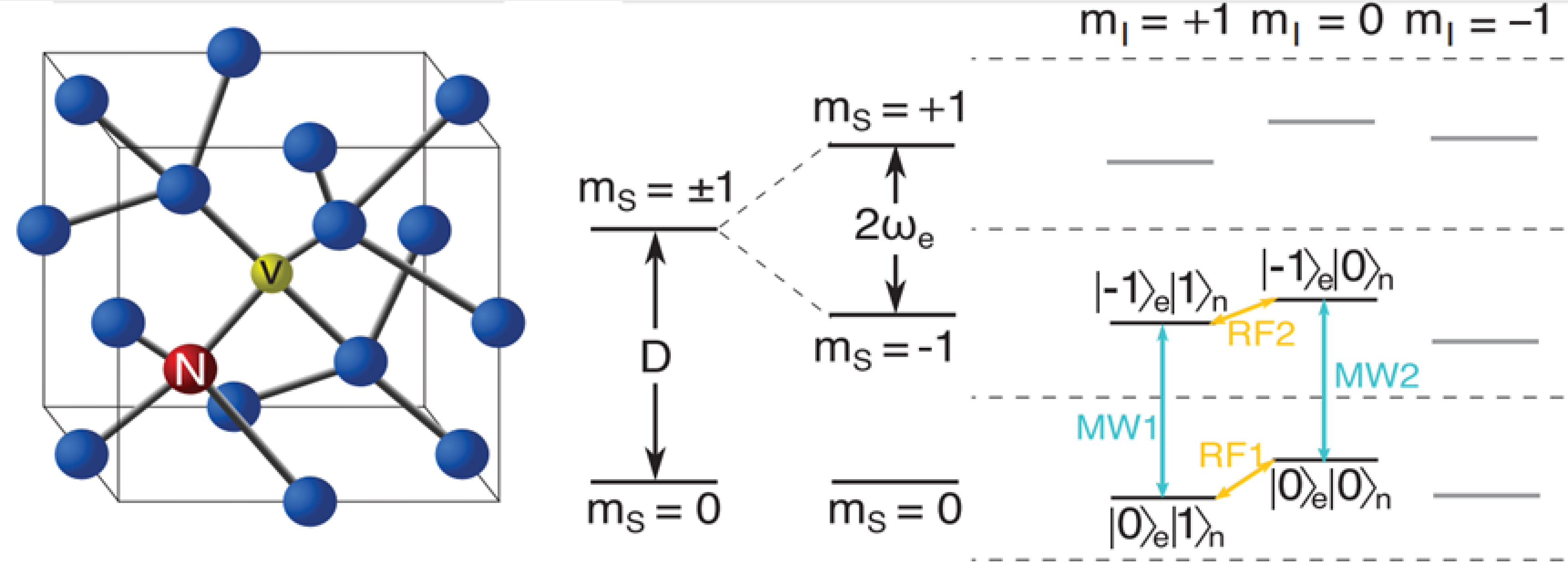
(Received 1 December 1997; revised manuscript received 9 April 1998)

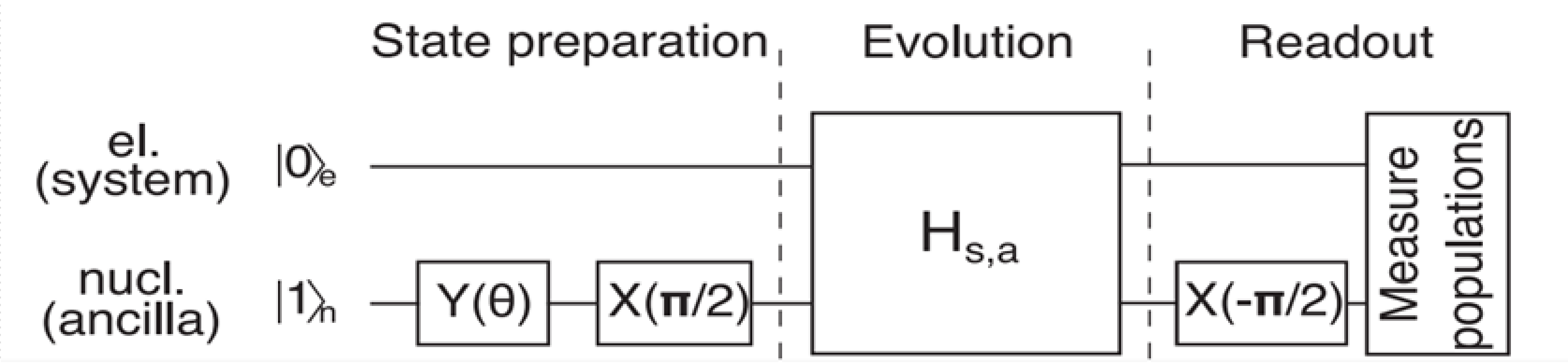
In 1998, Bender et al. proposed that a class of non-Hermit Hamiltonian satisfying PT -symmetry can still exhibit real eigenenergies.

Parity operator: $\mathcal{P}^2 = \mathbf{1}.$ Time reversal operator: $\mathcal{T}A\mathcal{T} = A^*$

PT symmetric Hamiltonian H_{PT}: $[\mathrm{H}_{\mathcal{PT}}, \mathcal{PT}] = 0$

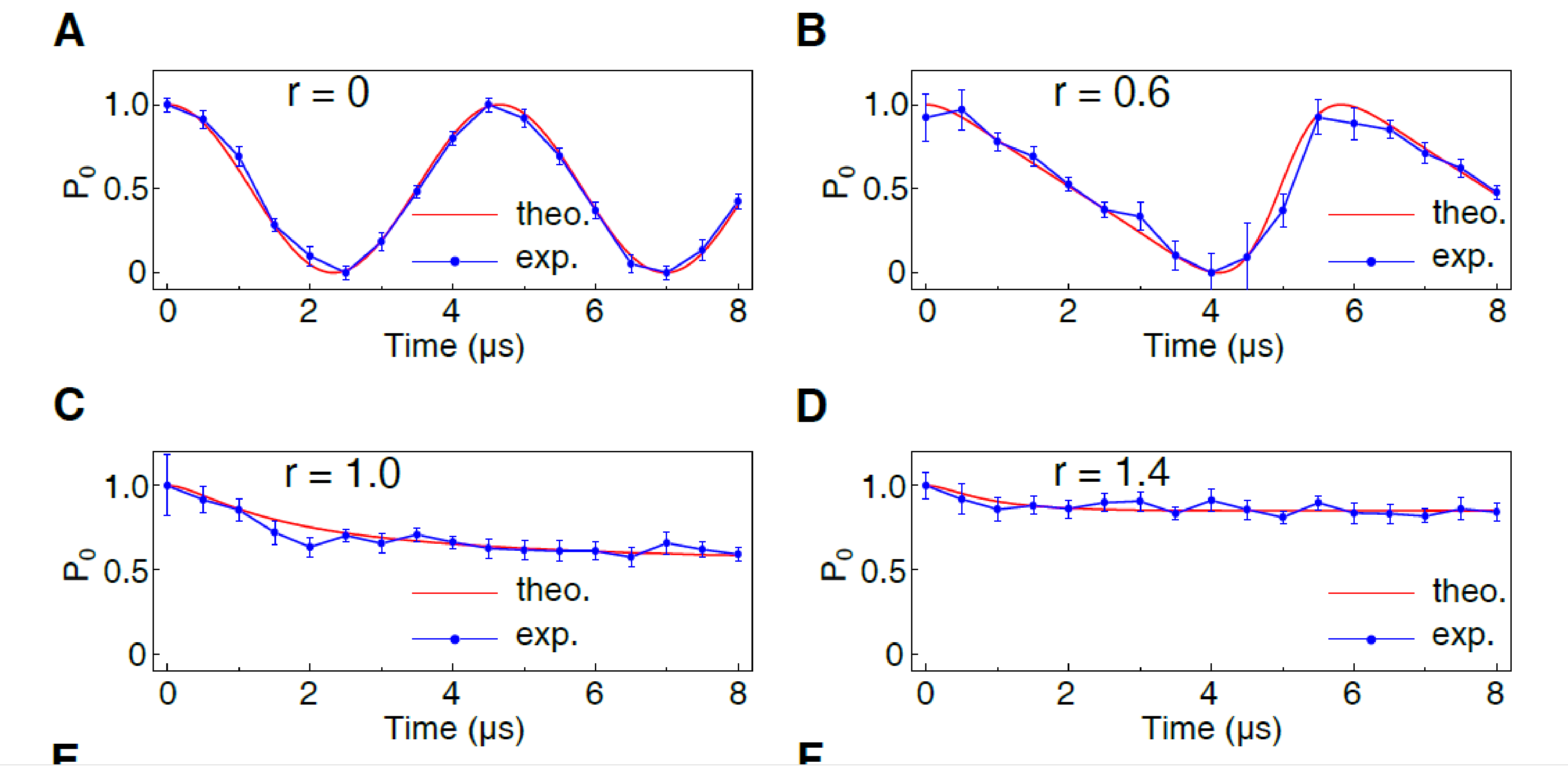
Realization of PT–symmetric Hamiltonian in an NV center





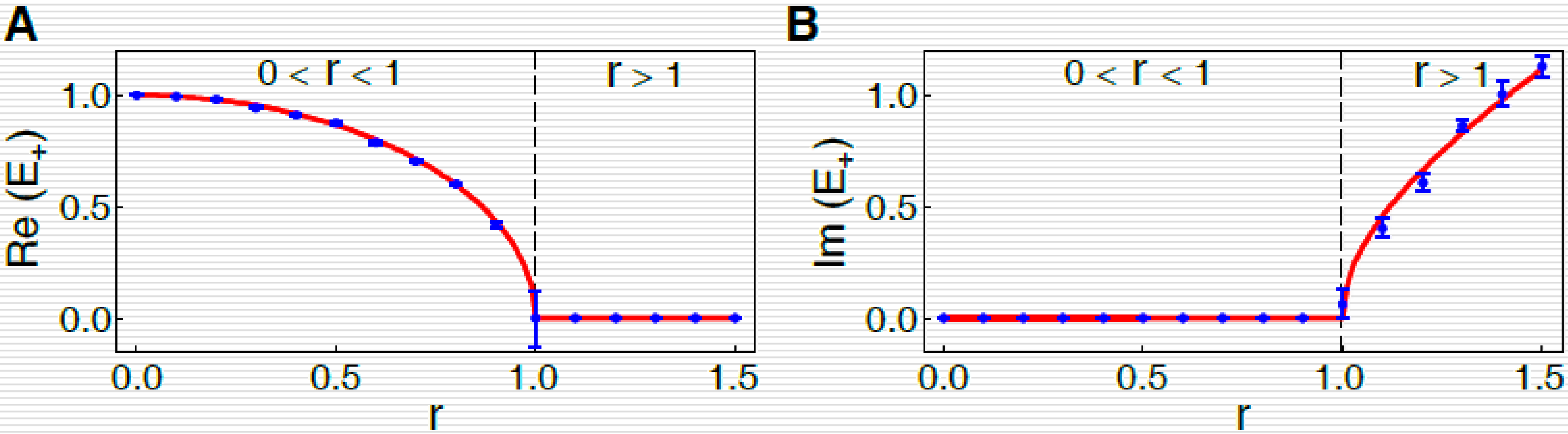
State dynamics under PT-Hamiltonian

$$H_s = \begin{bmatrix} ir & 1 \\ 1 & -ir \end{bmatrix}$$



Yang Wu et al., Science 364.878 (2019)

Observing the breaking of PT symmetry



$$E = \pm\sqrt{1 - r^2}.$$

$$H_s = \begin{bmatrix} ir & 1 \\ 1 & -ir \end{bmatrix}$$

- |r|<1: unbroken PT symmetry
- |r|>1: broken PT symmetry
- r = 1: Exceptional point

Yang Wu et al., Science 364.878 (2019)

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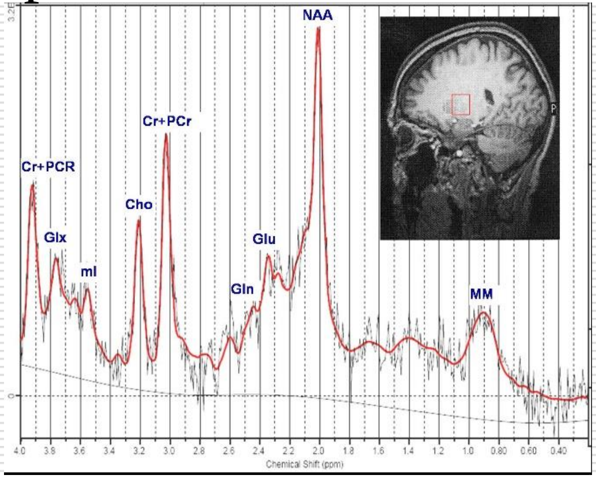
Ensemble magnetic resonance spectrometer

	Spins
NMR	10^{10}
ESR	10^{7}

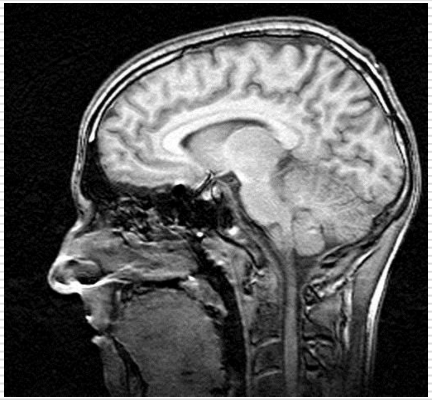
Volume of sample is cm ~ mm

Conversional NMR or ESR spectrometers collect the signal from spin ensembles (more than billions). This technology has been used on physics, chemistry, biology, medicine and so on.

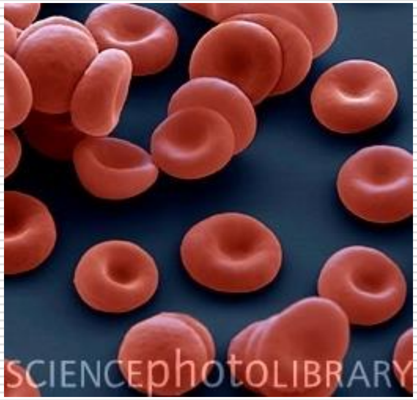


Trend of science and technology

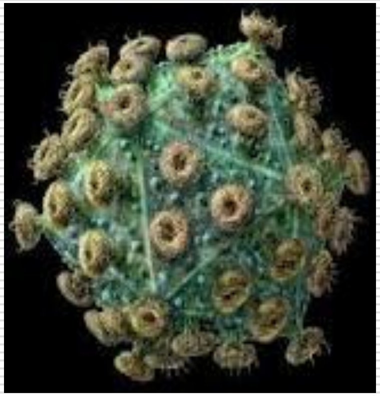
Macro



Human’s brain



Red blood cell



HIV

DNA

Micro

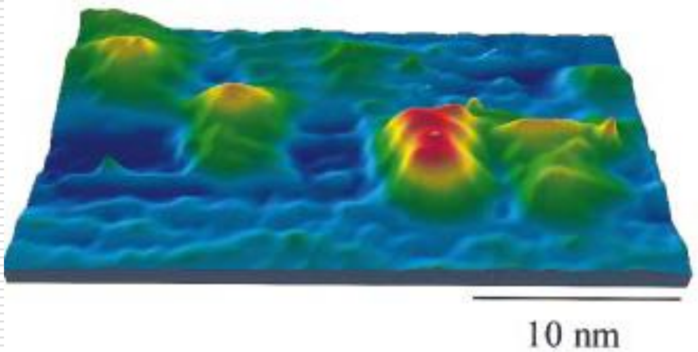
10 mm 10 μm 10 nm 1 nm

- Nanoscale magnetic resonance enables detection of elements, structure and dynamics behavior on nanoscale even single molecule.

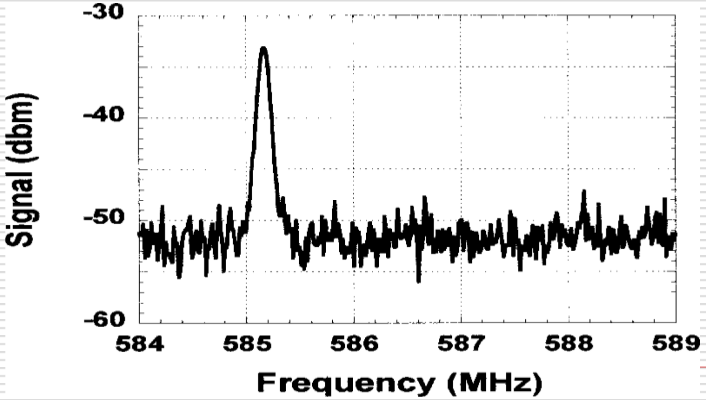
Single electron had been detected under ultra-low temperature

VOLUME 62, NUMBER 21 PHYSICAL REVIEW LETTERS 22 MAY 1989

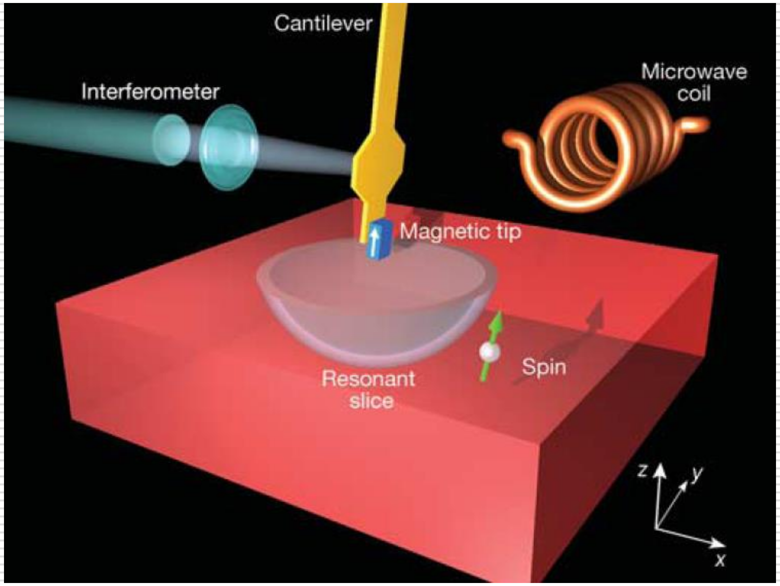
Direct Observation of the Precession of Individual Paramagnetic Spins on Oxidized Silicon Surfaces



STM-ESR
PRL, 1989
APL, 2002



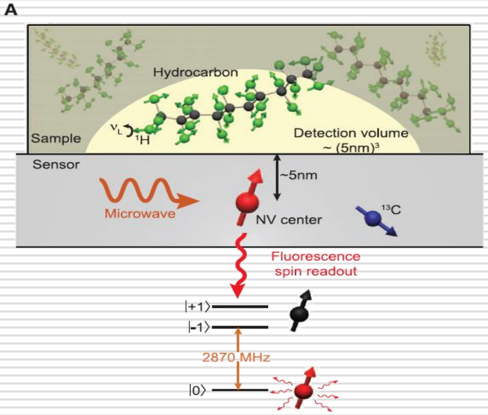
MRFM
Nature
2004



MR: ensemble to single molecule under ambient conditions

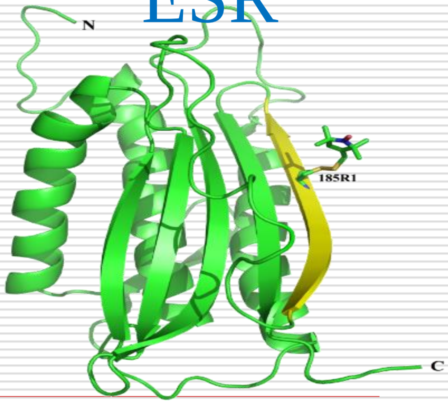
- Quantum control on NV

Enables nanoscale



NMR

ESR



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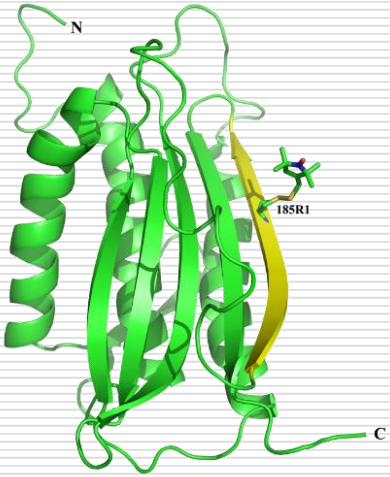
Samples

Large ensembles

~ **10^{16}**

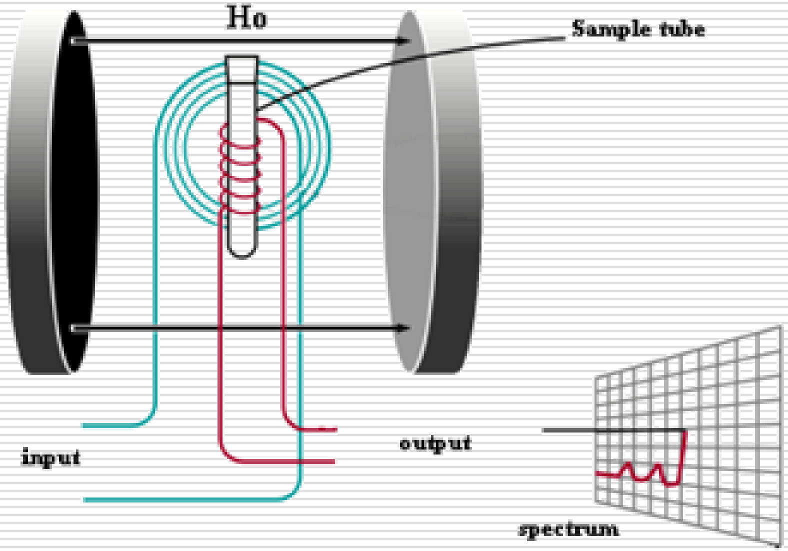


Nanoscale

Even single spin

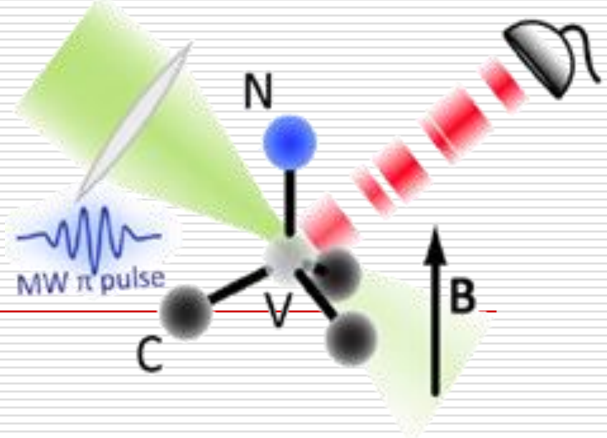
volumn	cm ~ mm	nm
Spins	10^{16}~10^{10}	10^{5}~10^{0}

Detection methods



Probe	Coil/cavity	NV
Signal	Current	Phase of qubit
Technology	Electronic	Quantum control

NV center in diamond



Consist of a substitutional Nitrogen atom and an adjacent Vacancy. (named NV defect center)

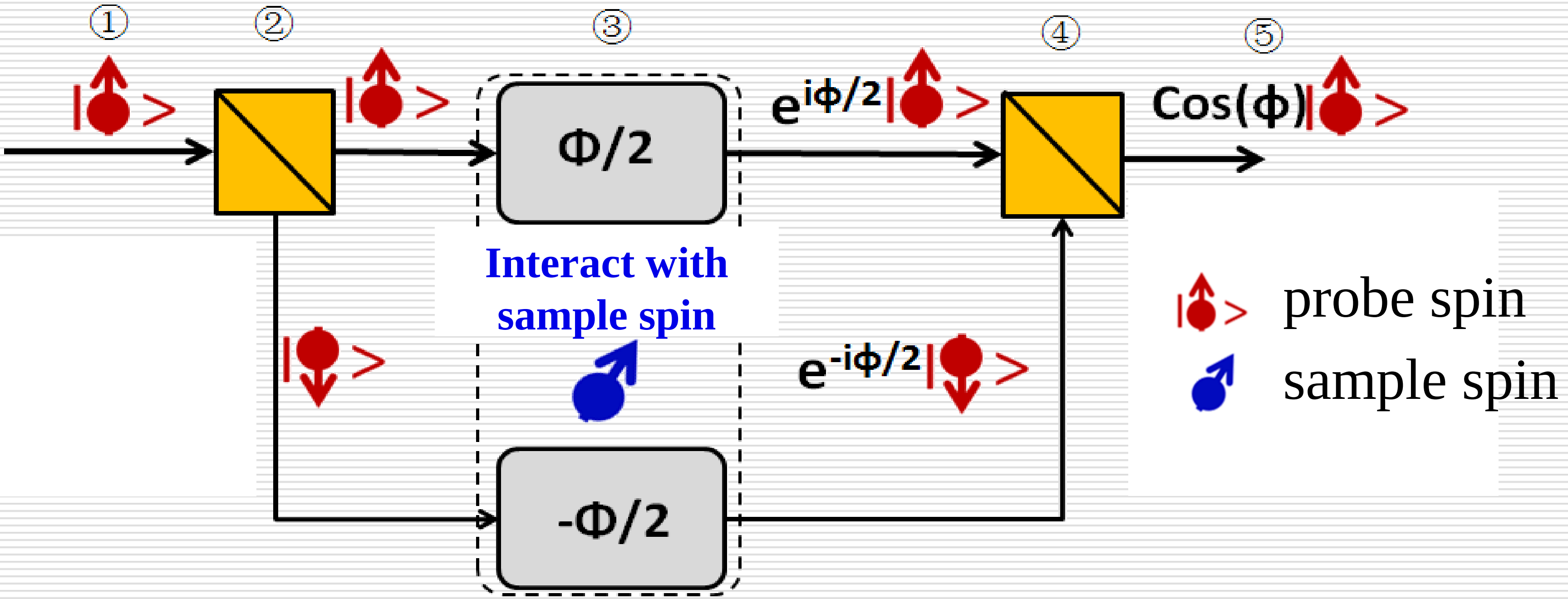
One of outstanding defects in diamond.

Amazing features:

- Optical detection of the spin state
- Optical spin polarisation of the ground state (« Laser cooling »)
- Narrow lines, $T_2 > 1$ ms @ RT

The working principle of NV sensor

Using single-spin quantum interferometer to convert the weak magnetic signal to the measurable spin quantum phase

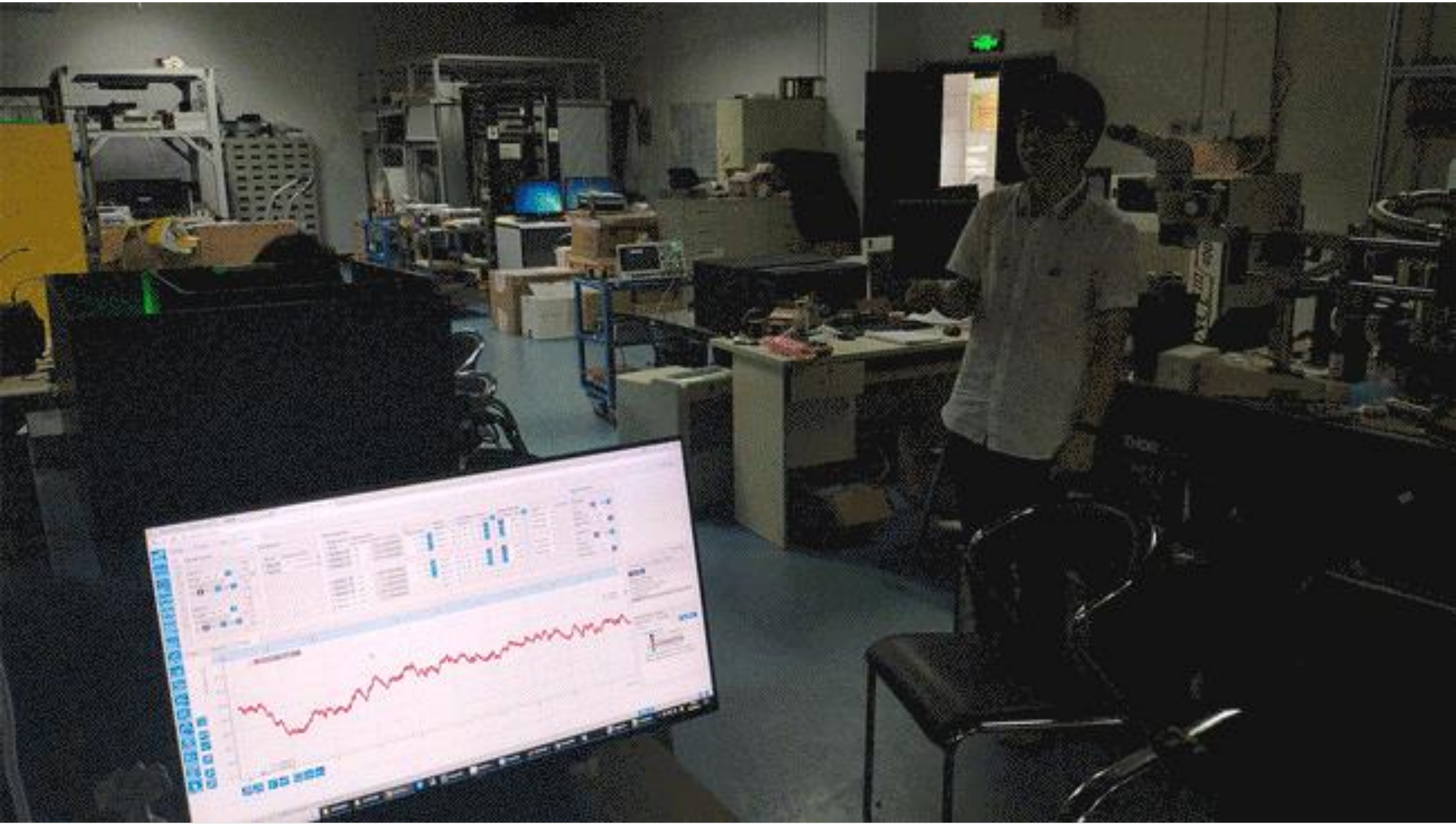


① Initial state preparation
② Generate quantum superposition
③ Accumulate quantum phases
④ Interfere of the quantum states
⑤ Readout

$$\Phi \propto \eta \cdot t$$

η the strength of coupling

t the detecting time, *limited by the quantum coherence time of probe spin*



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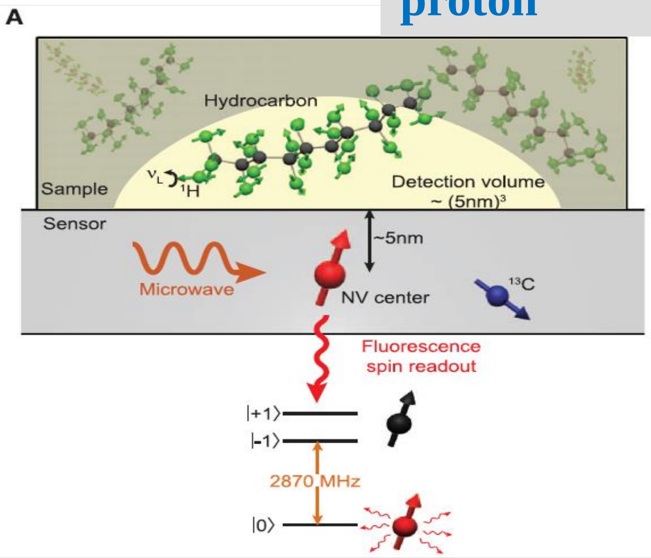
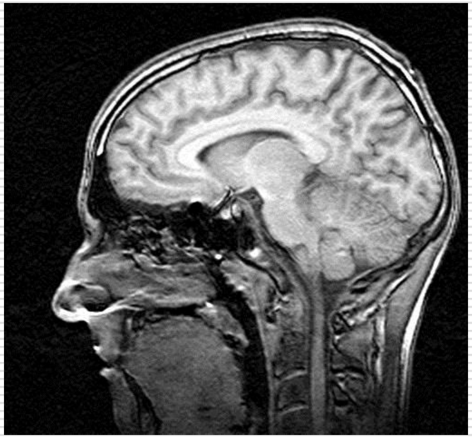
NMR: millimeters to nanometers

~ mm

~ 5nm spectrum

proton

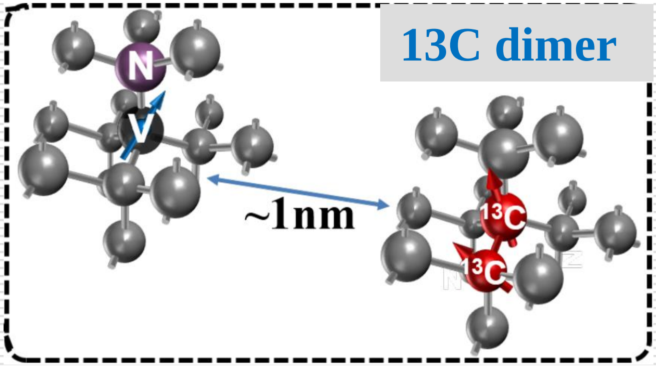




Conventional MR
(10^{10}~10^{19} Spins)

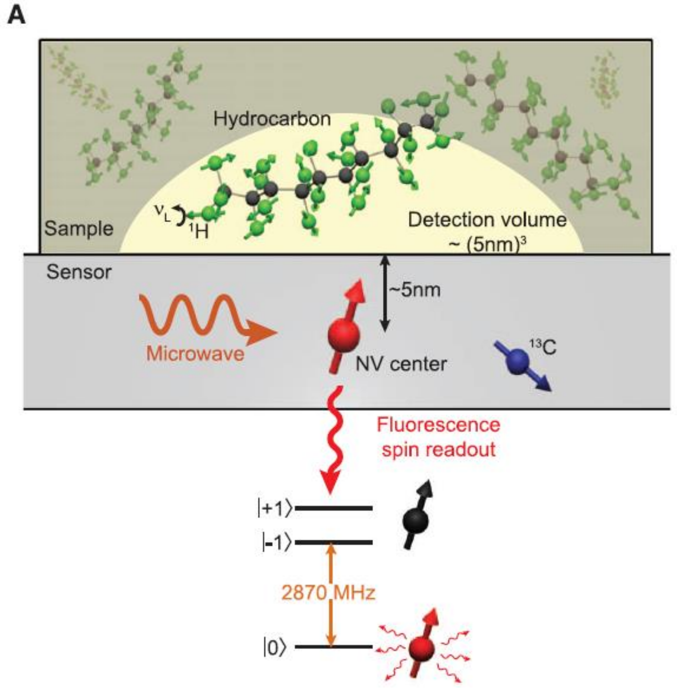
~ atomic-scale structure analysis

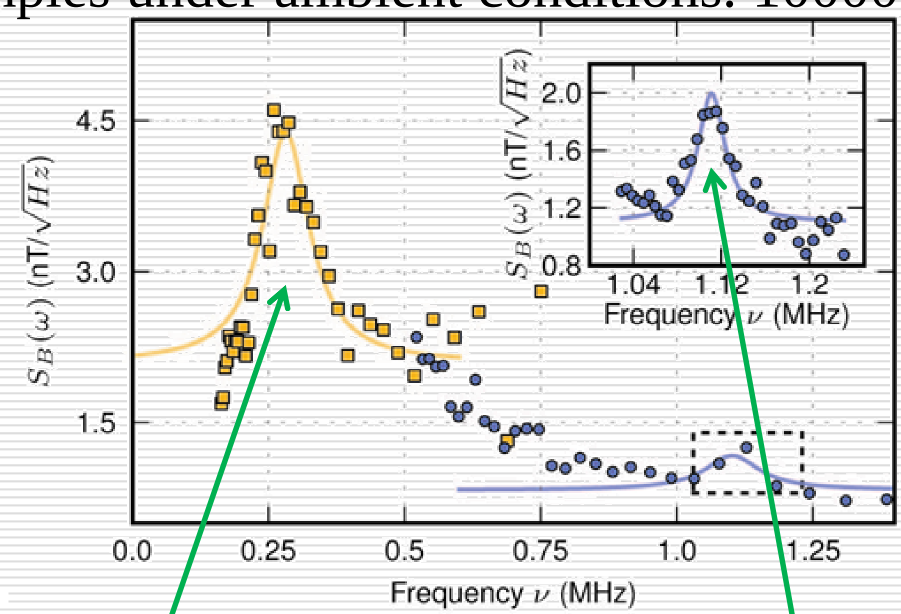
13C dimer



1. Nano-NMR spectrum

We demonstrated detection of NMR signals from a (5-nanometer)^3 voxel of various fluid and solid organic samples under ambient conditions. 10000 protons were included.





strong contribution of ^{13}C nuclei inside the diamond (CPMG6)

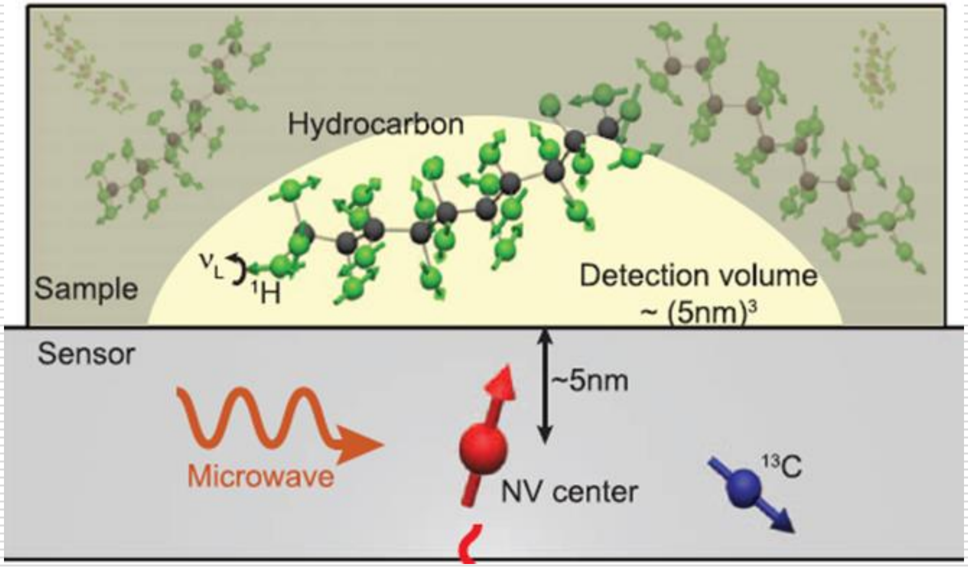
a weaker component of ^{1}H nuclei of the sample of microscopy immersion oil (XY8-160)

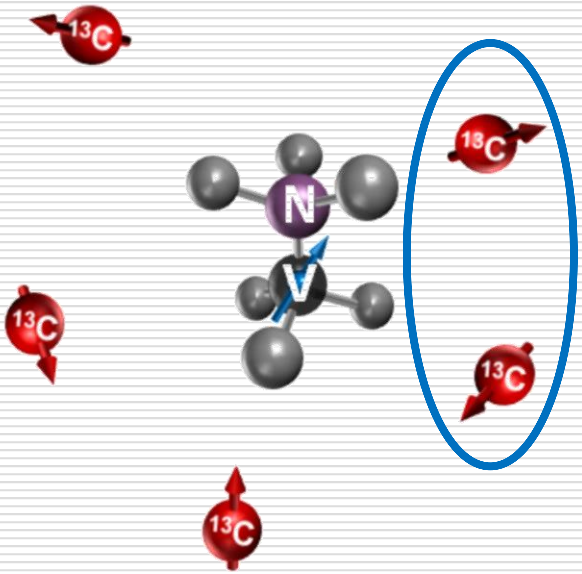
T. Staudacher, F. Shi et al., Science 339, 561 (2013)

2. Structure analysis of single nuclear spin dimer

Individual proton spins

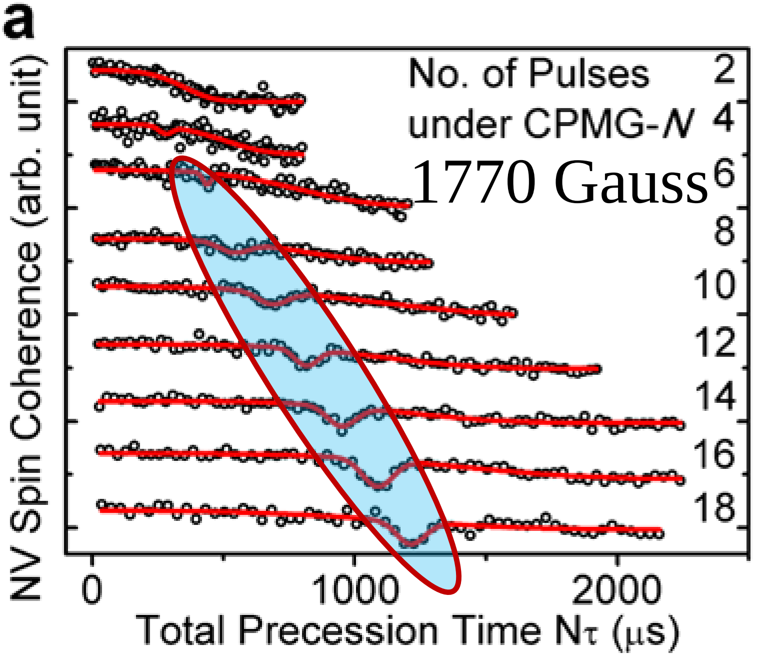
Interact carbon-13 spins



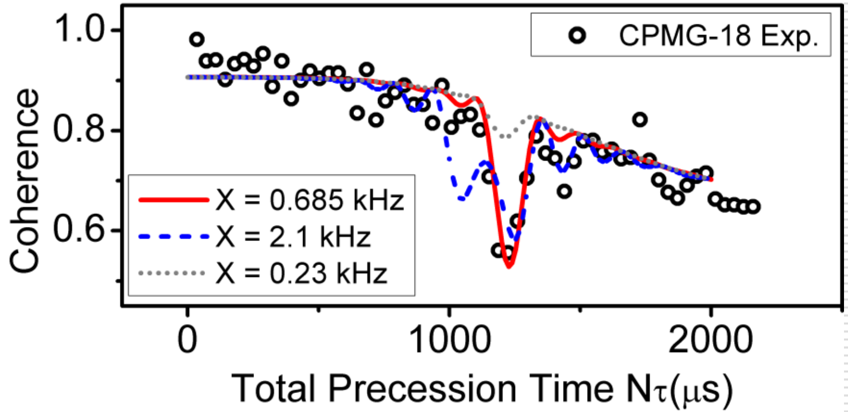


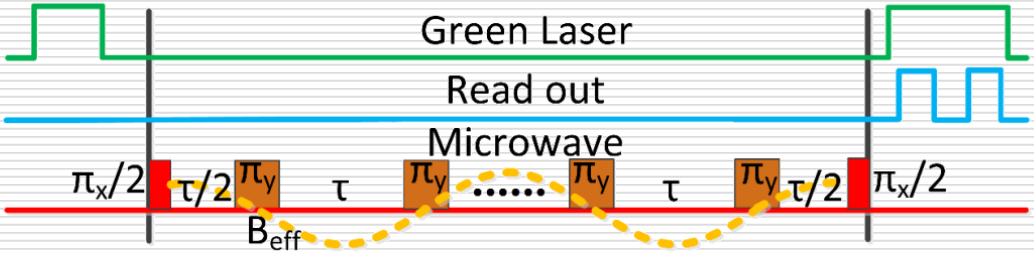
Directly measuring interactions within single nuclear spin clusters are used for structure analysis.

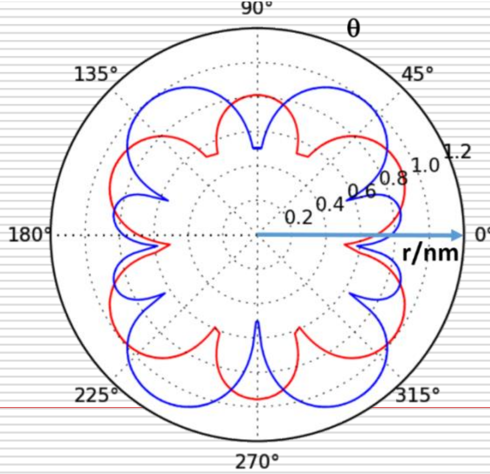
2. Structure analysis of single nuclear spin dimer



a ^{13}C-^{13}C dimer was detected.





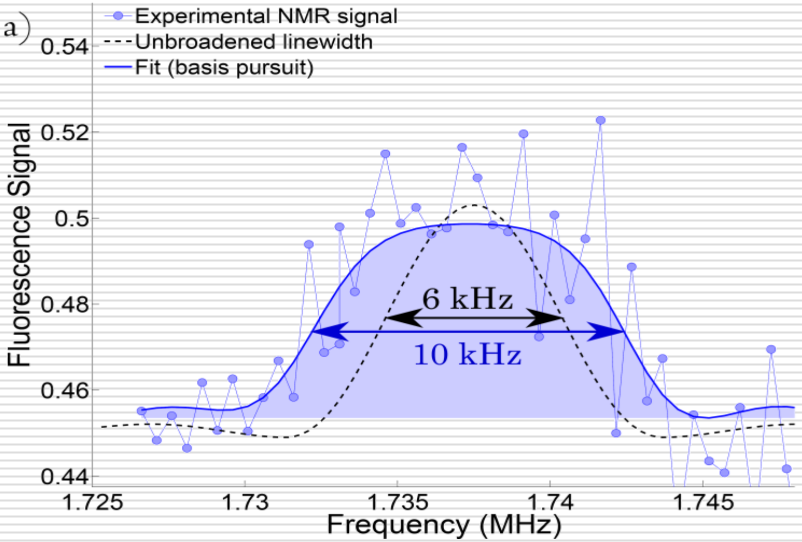


F. Shi et al., Nature Physics 10, 21 (2014)

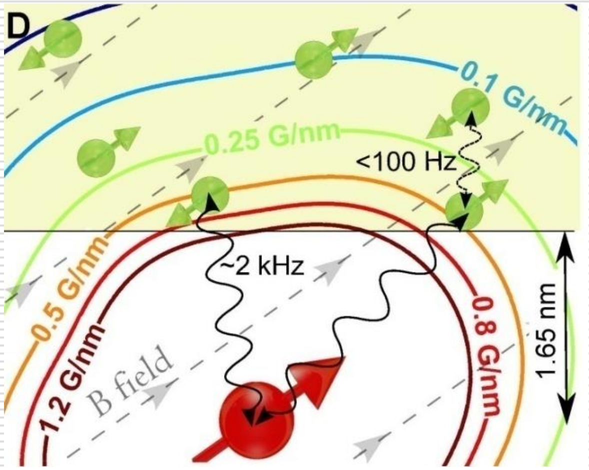
3. NMR with single proton spin sensitivity

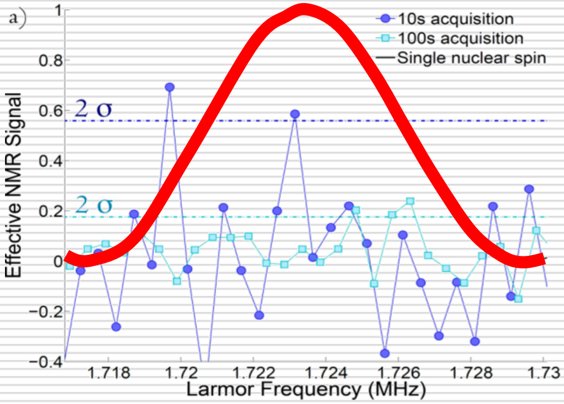
NMR of four ^{29}Si nuclear spins;

Effective single proton spin sensitivity.



4 ^{29}Si spin NMR spectrum





C. Mueller, X. Kong, et al., Nature Communications 4, 3704 (2014)

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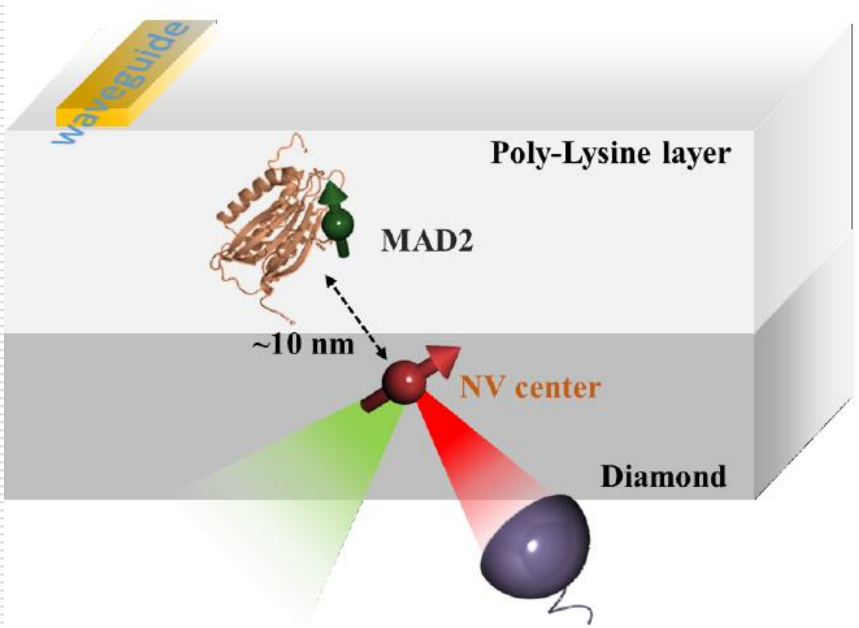
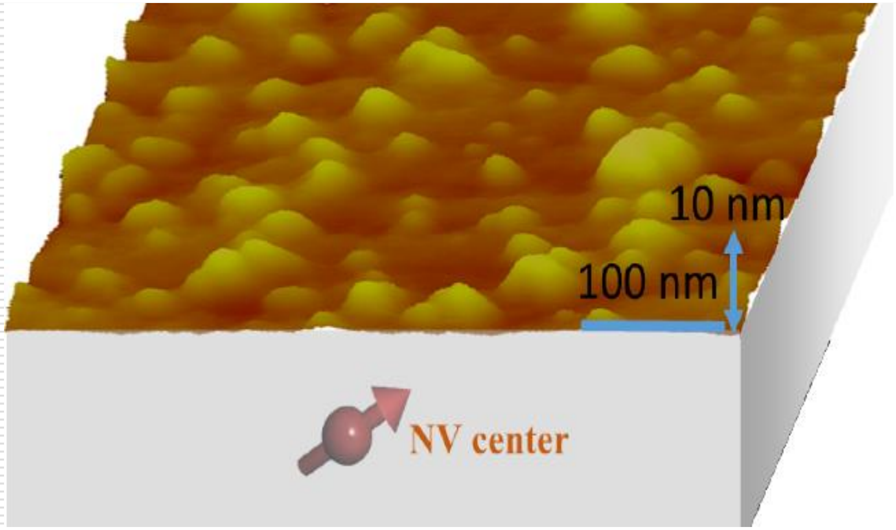
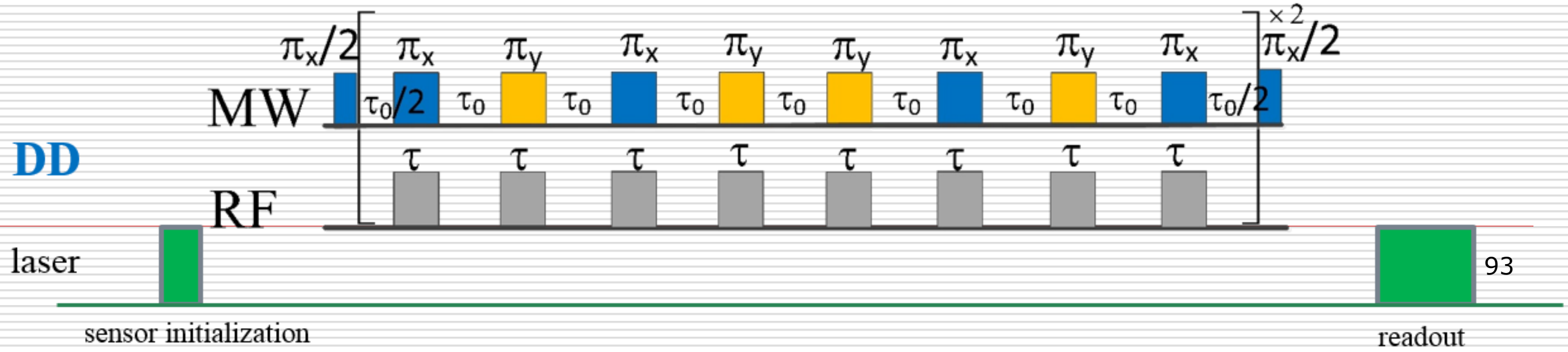
Single protein ESR:
Experimental setup and detecting method



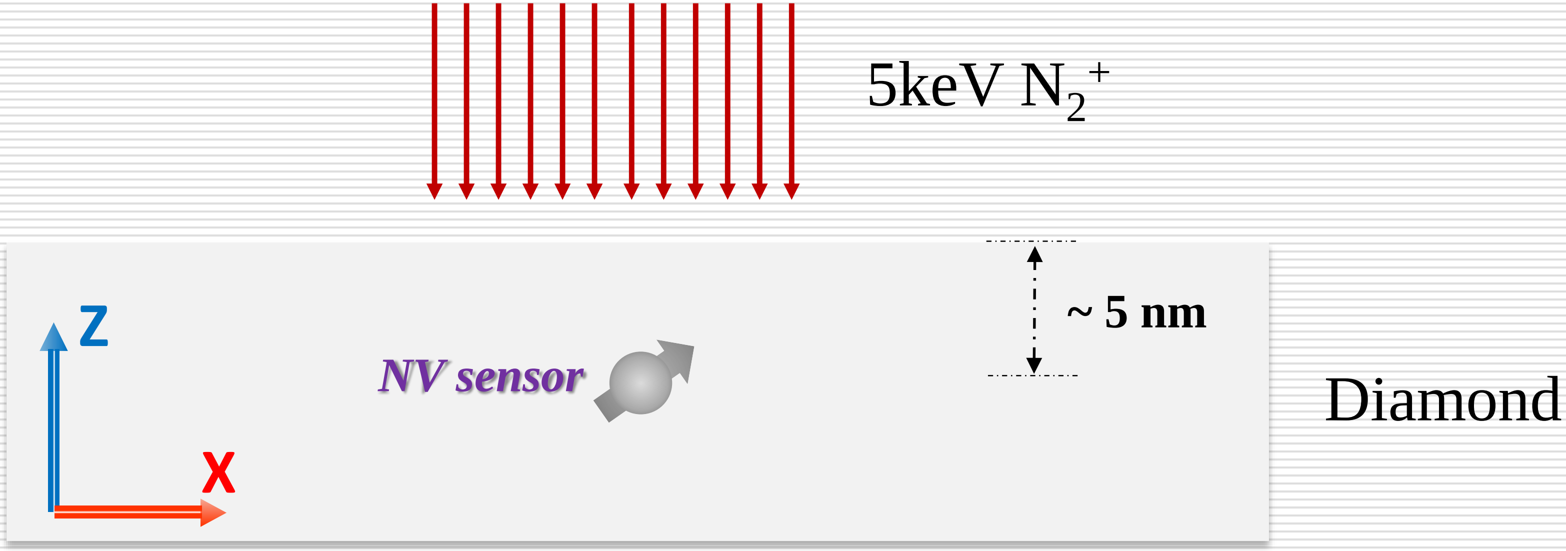


Fazhan Shi et al., **Science** 347, 1135 (2015).

DEER + DD

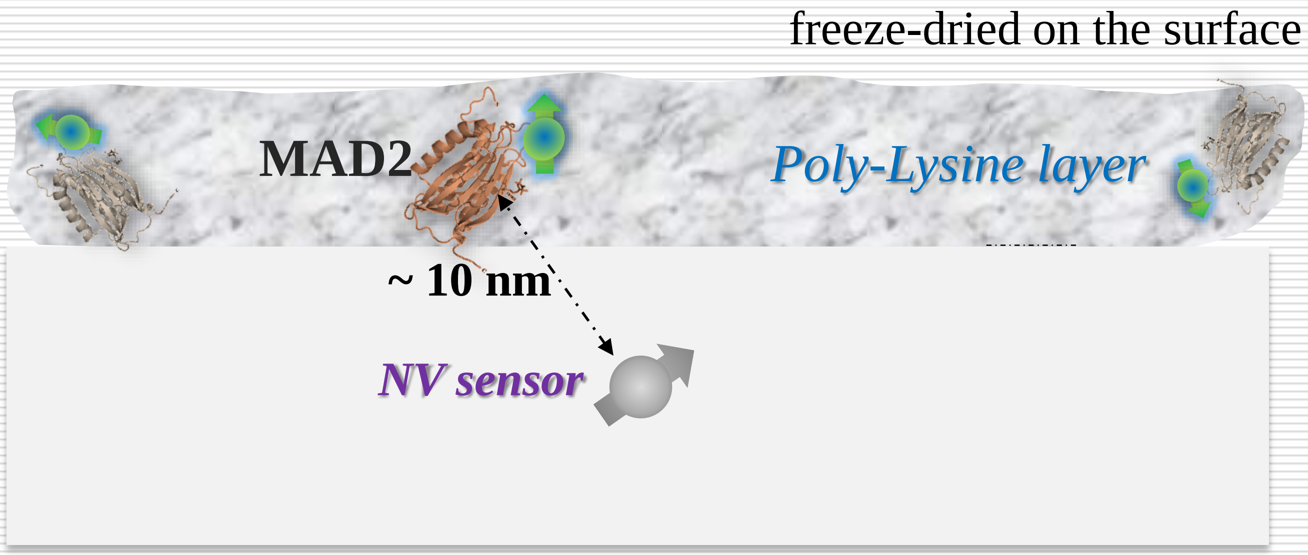


Controls on NV sensor and label spin



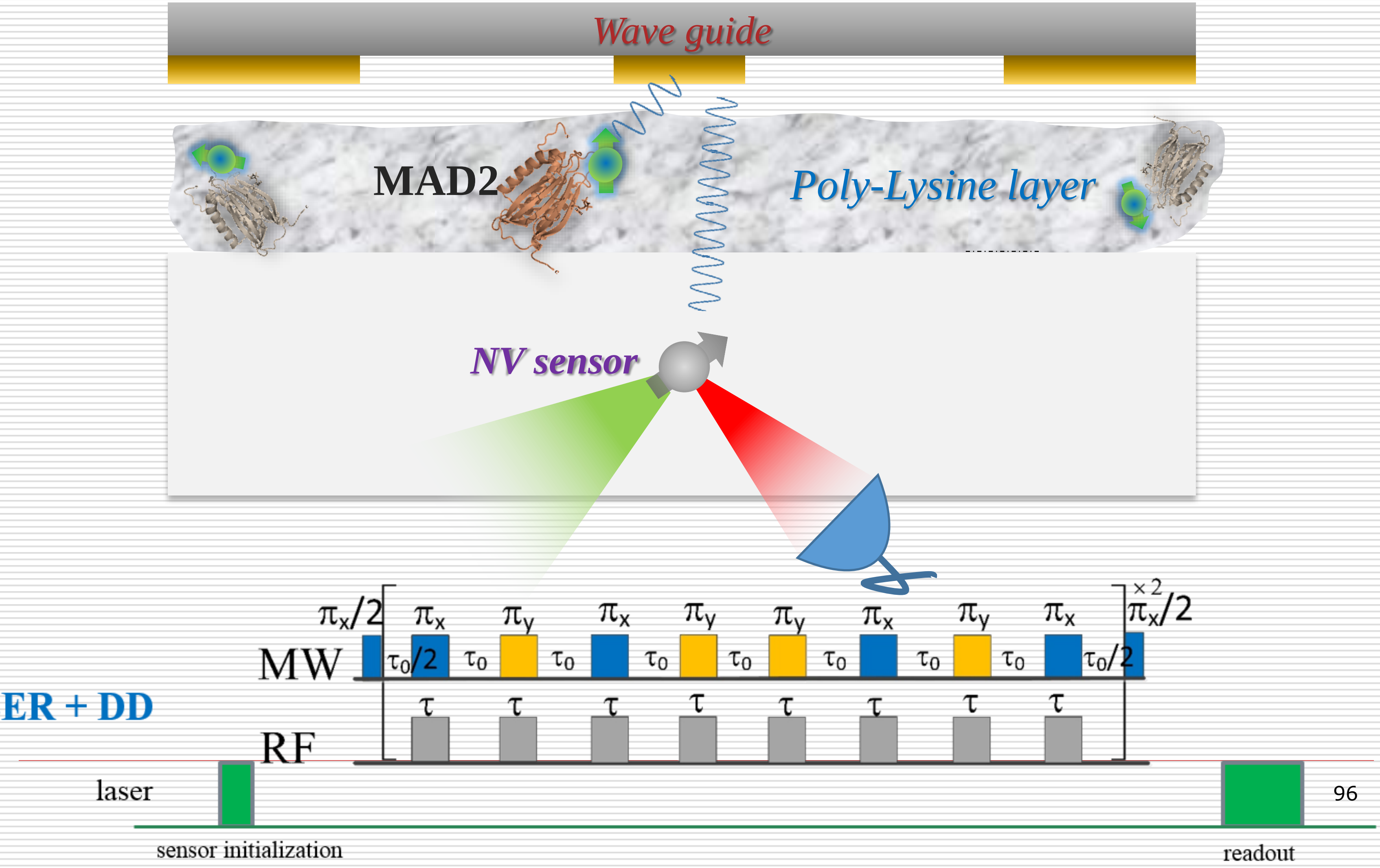
Fazhan Shi et al., **Science** 347, 1135 (2015).

Controls on NV sensor and label spin



Fazhan Shi et al., **Science** 347, 1135 (2015).

Controls on NV sensor and label spin

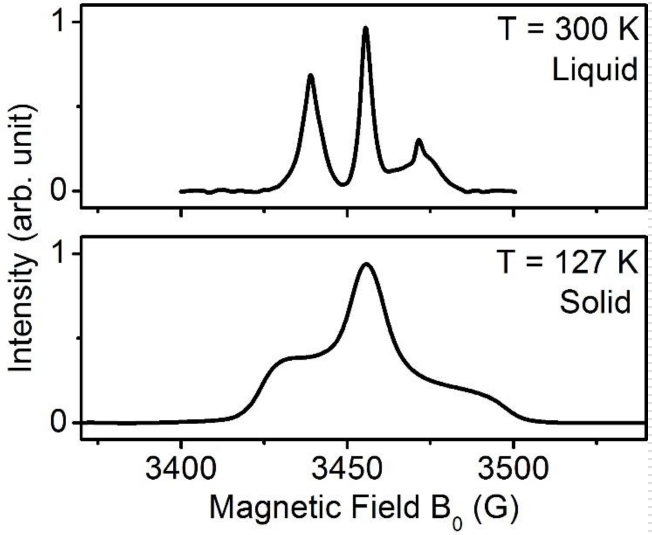


DEER + DD

Single protein ESR:
CW spectrum of nitroxide spin labels

Liquid ESR

~ 10^{16} protein molecules
water solution @ 300K.

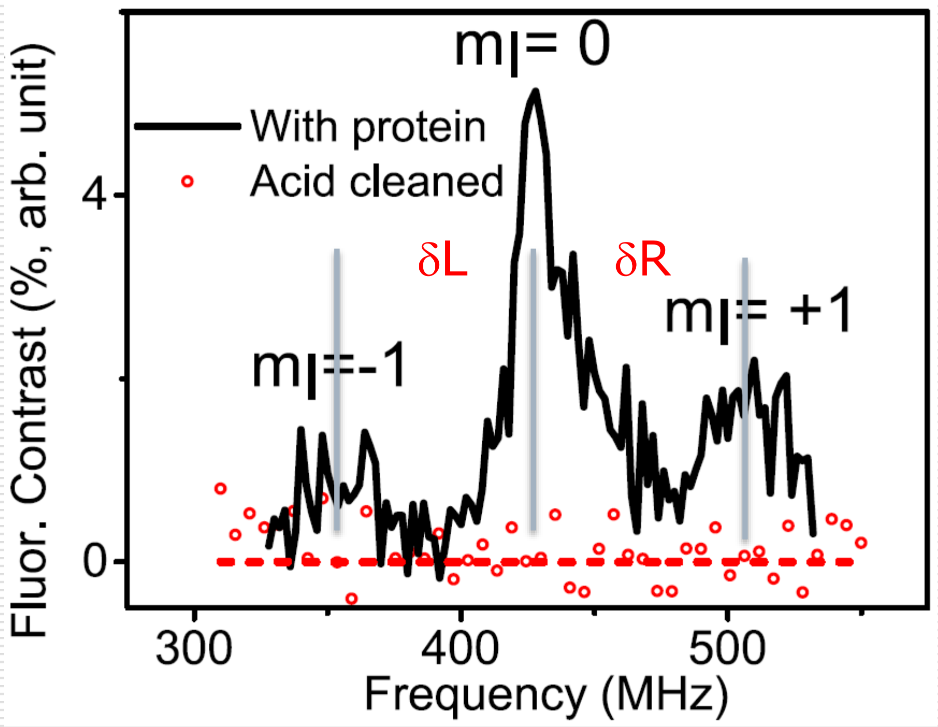


Solid ESR

~ 10^{15} protein molecules
water solution (ice) @ 127K.

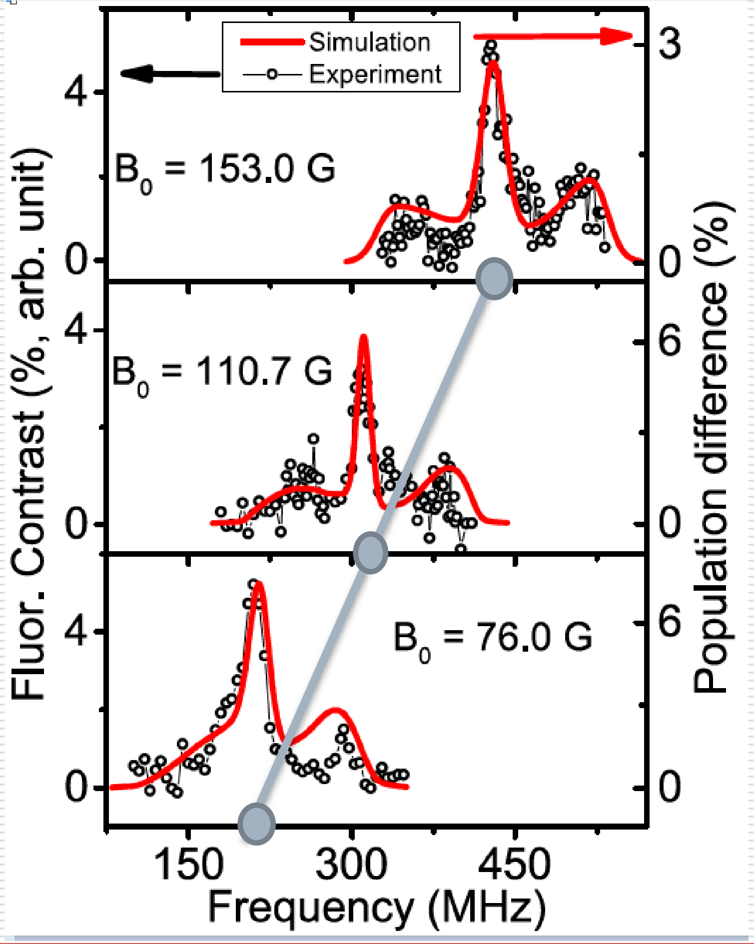
Single molecule spectrum

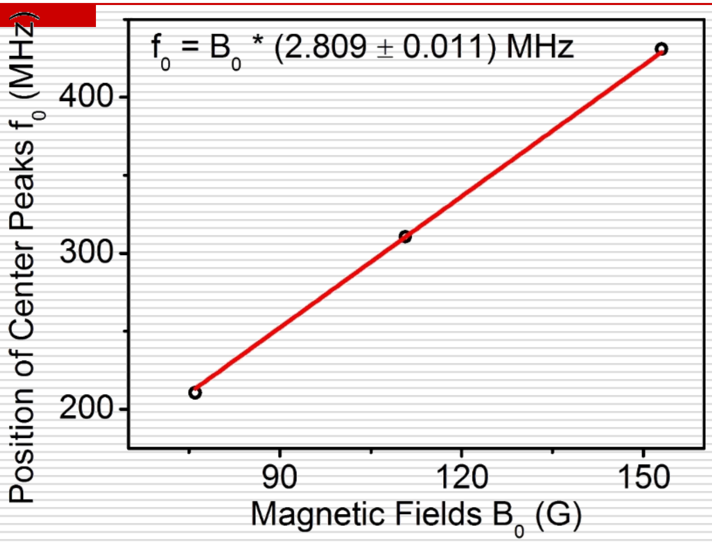
with/without protein on surface



Fazhan Shi et al., **Science** 347, 1135 (2015).

Single protein ESR:
g-factor from CW spectrum





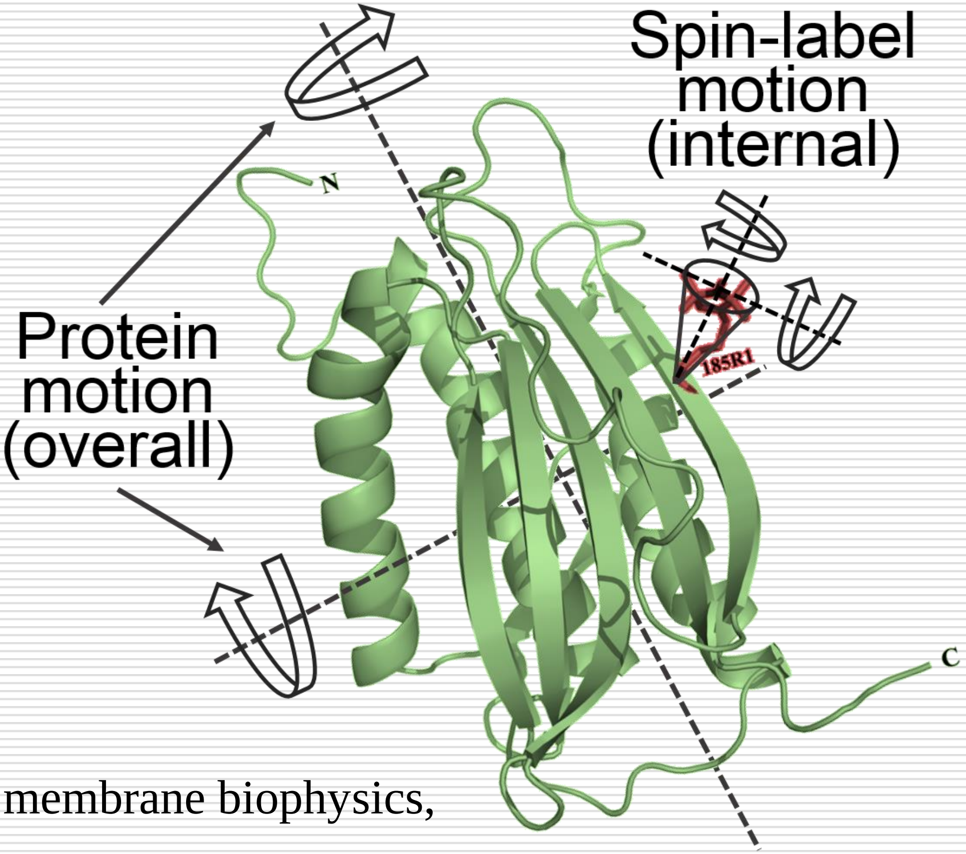
$$f_0 = \gamma_e B_0 = g\,\mu_B\,B_0$$

$$\gamma_e = 2.809 \pm 0.011 \text{ MHz/G}$$

$$\Rightarrow g = \gamma_e / \mu_B$$
$$= 2.008 \pm 0.006$$

Fazhan Shi et al., **Science** 347, 1135 (2015).

Protein Motions



timescale
~ nanosecond

Biophysics
88, 4351 (2005)

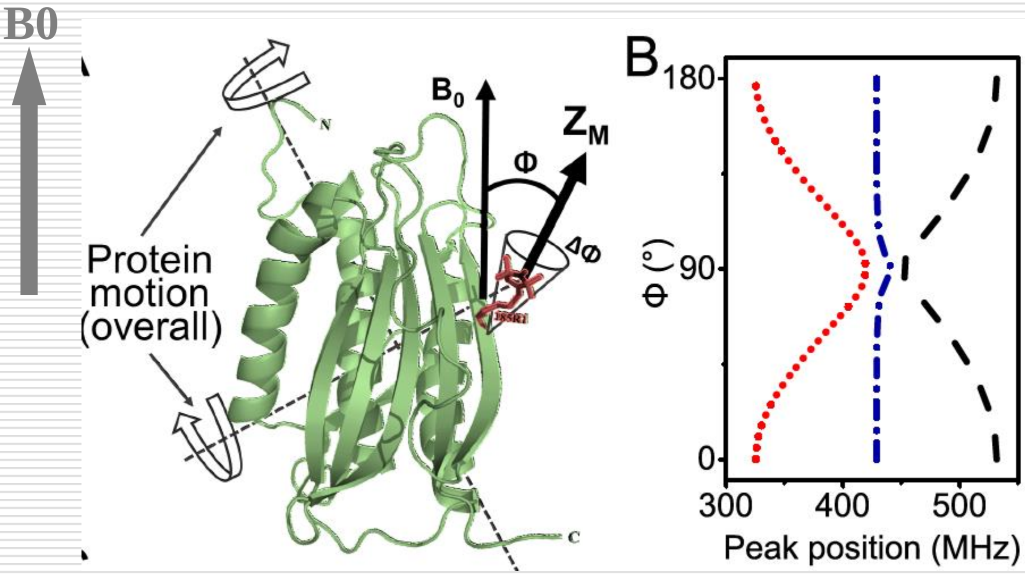
timescale
~ millisecond

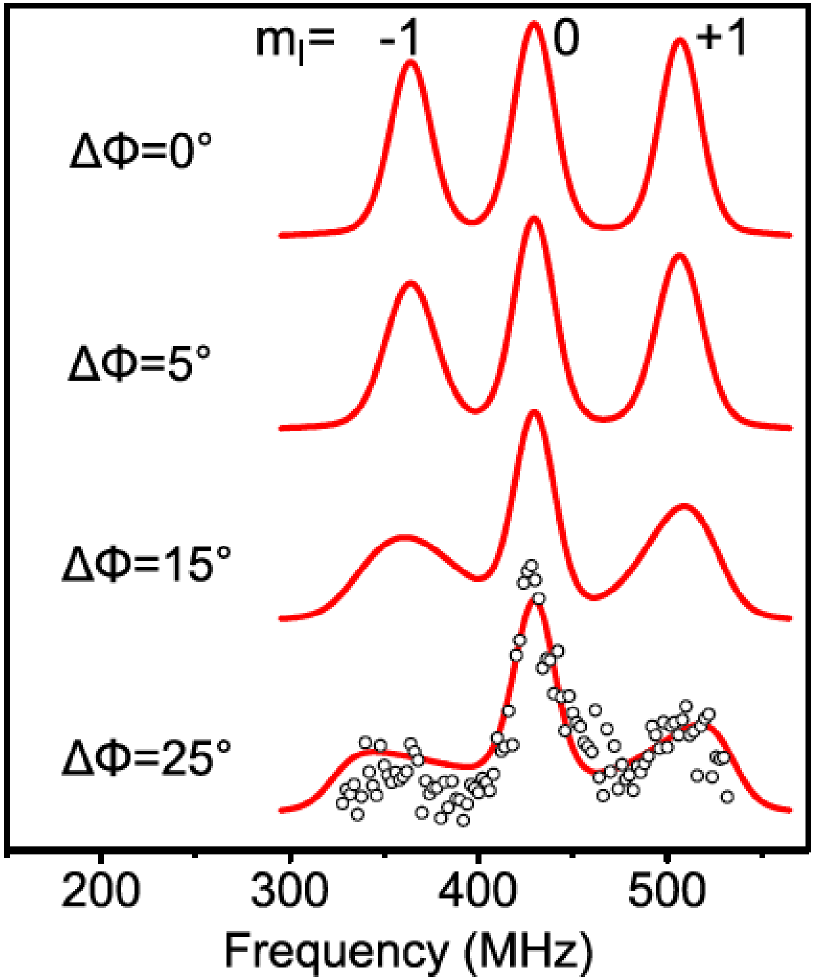
ESR spectroscopy in membrane biophysics, pp 133-134, 2007

Fazhan Shi et al., **Science** 347, 1135 (2015).

Target spin motion

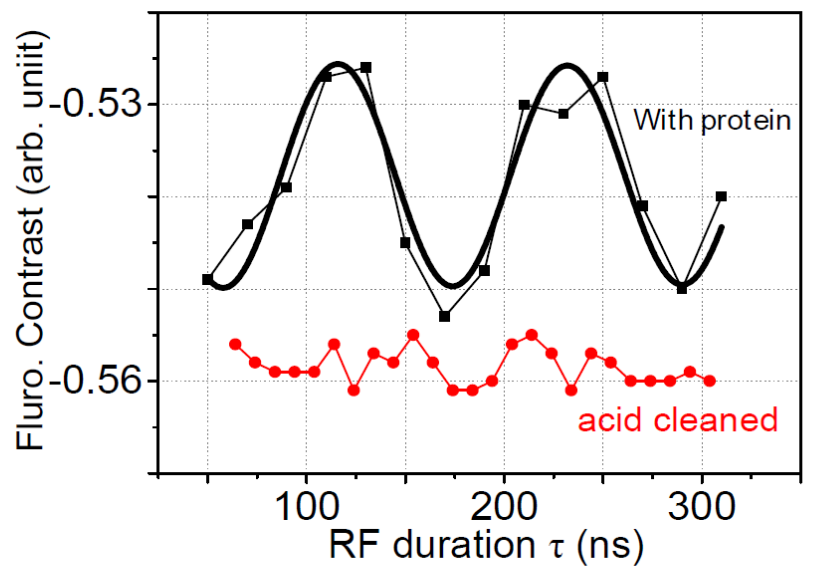
The shape of spectra depends on the overall motion, i.e., (Φ, ΔΦ)





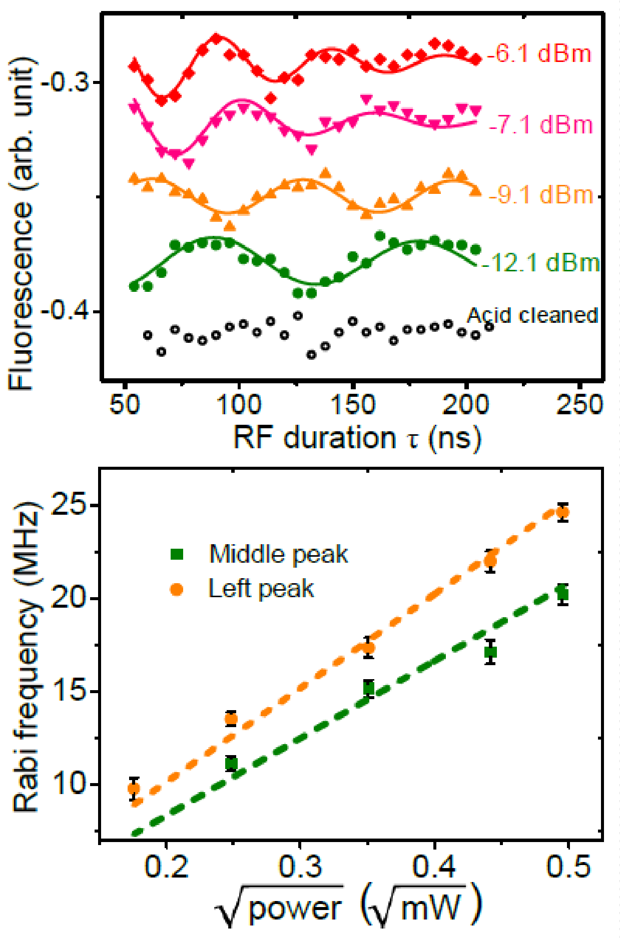
Fazhan Shi et al., **Science** 347, 1135 (2015).

Quantum manipulation on protein spin



Rabi oscillation with/without proteins on the diamond surface.

The Rabi frequency linearly depends on Square root of microwave power.

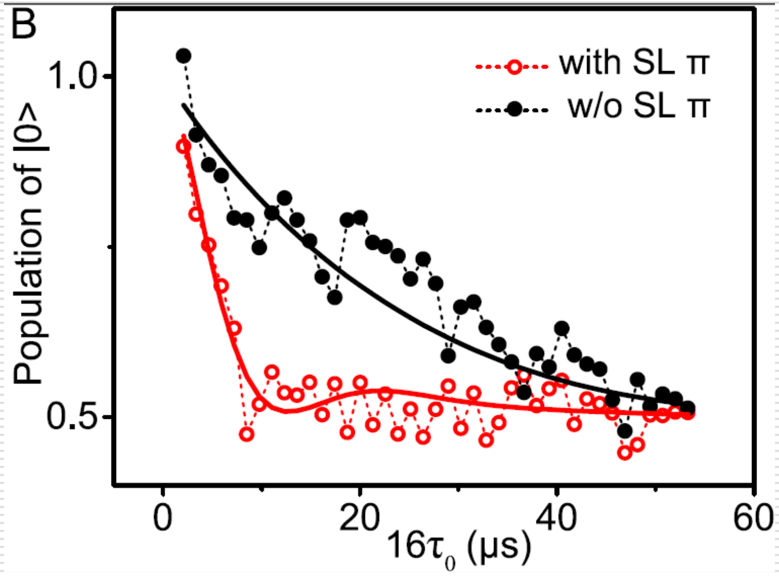


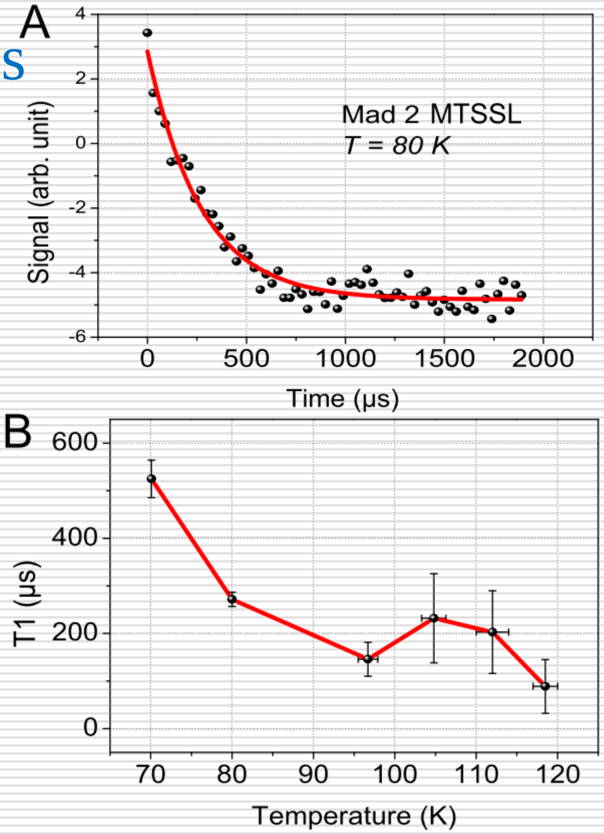
Fazhan Shi et al., **Science** 347, 1135 (2015).

relaxation time of

single protein

ensemble proteins



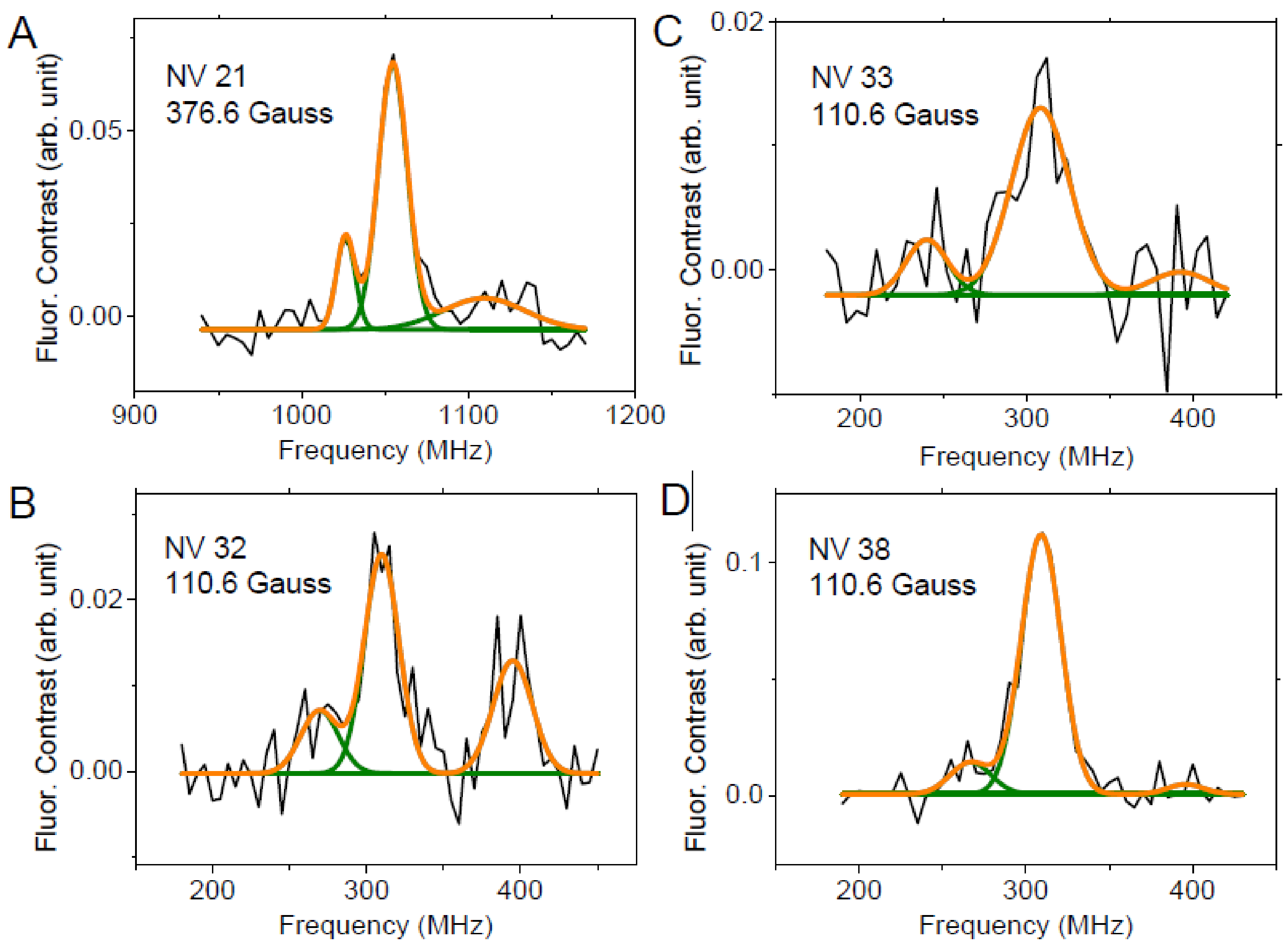


Relaxation time is roughly 4 us.

$$T_{1,\mathrm{MTSSL}} \approx 0.29\ \mu s$$

Fazhan Shi et al., **Science** 347, 1135 (2015).

Reproduce the spectra on other NV sensors

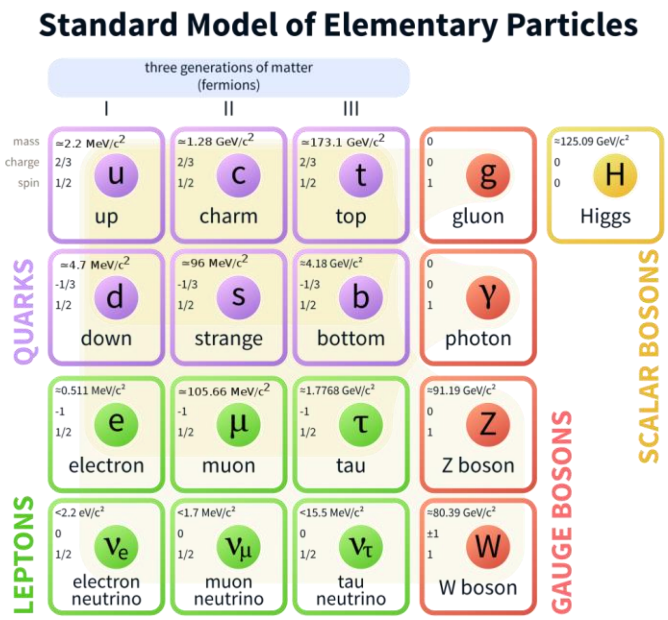


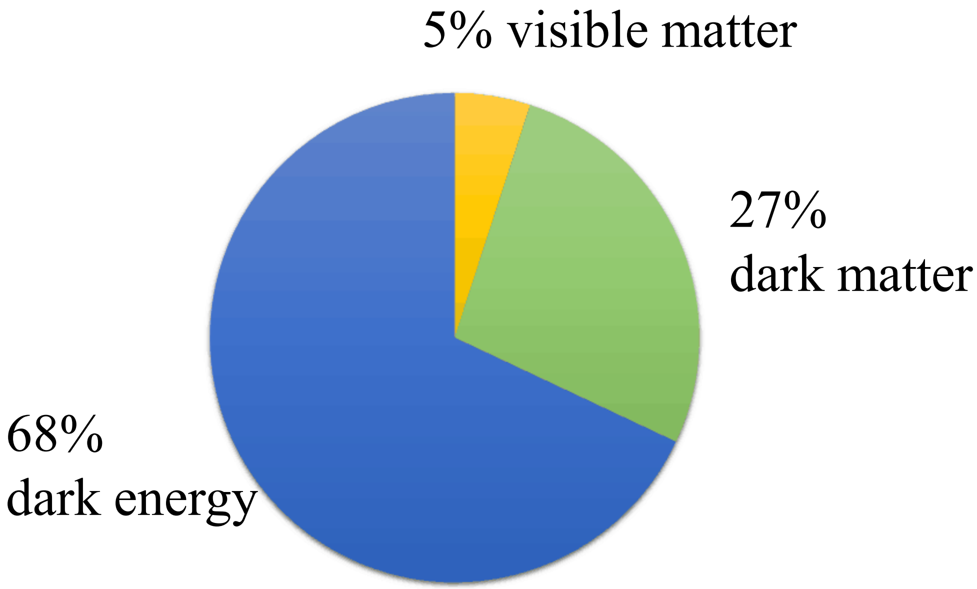
Outlines

- ☐ Introduction
- ☐ Quantum Computations
- ☐ Quantum Simulations
- ☐ Quantum Sensing:
  - ➢ Background
  - ➢ NV sensor – setups and detecting method
  - ➢ Progresses in nanoscale NMR
  - ➢ ESR spectroscopy of single protein
  - ➢ Dark Matter Searching

研究背景

Science杂志 125个最具挑战性科学问题1号问题:
宇宙是什么构成的?

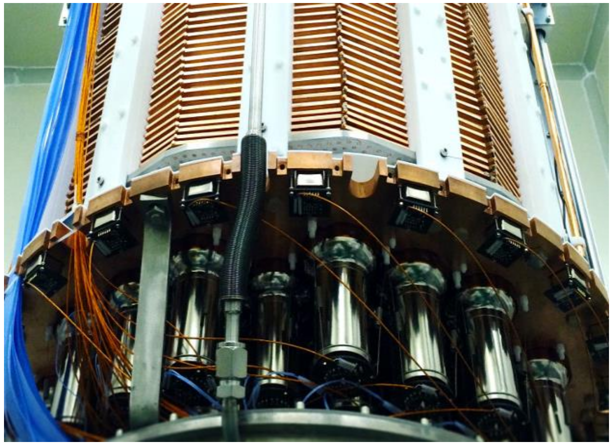




- 标准模型可以描述目前发现的基本粒子
- 宇宙仍有大部分物质是标准模型无法描述
- 研究超越标准模型新物理成为重要科学前沿

研究超越标准模型的新物理：搜寻（类）轴子

（类）轴子这类新粒子被提出用于解决标准模型无法解释的重要问题，是暗物质的重要候选者。搜寻（类）轴子是成为粒子物理的重大研究内容。



大型对撞机： LHC

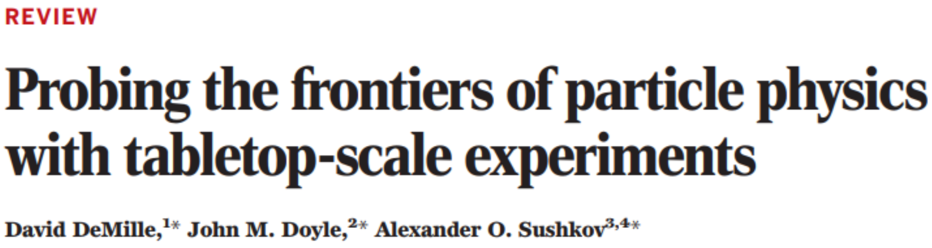
天文学观测： CAST

隶属于欧洲核子研究组织 CERN
(80个国家，约7000名科学家和工程师）

地下实验室：

- PANDAX (中国,$15 million)
- LUX (美国,$10 million)

新研究趋势——小型实验装置



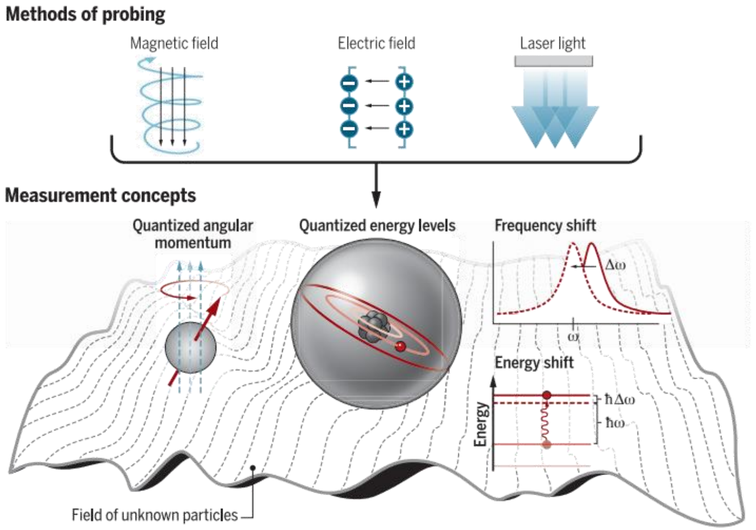
REVIEW

Probing the frontiers of particle physics with tabletop-scale experiments

David DeMille,[1*] John M. Doyle,[2*] Alexander O. Sushkov[3,4*]

DeMille et al., **Science** 357, 990–994 (2017)

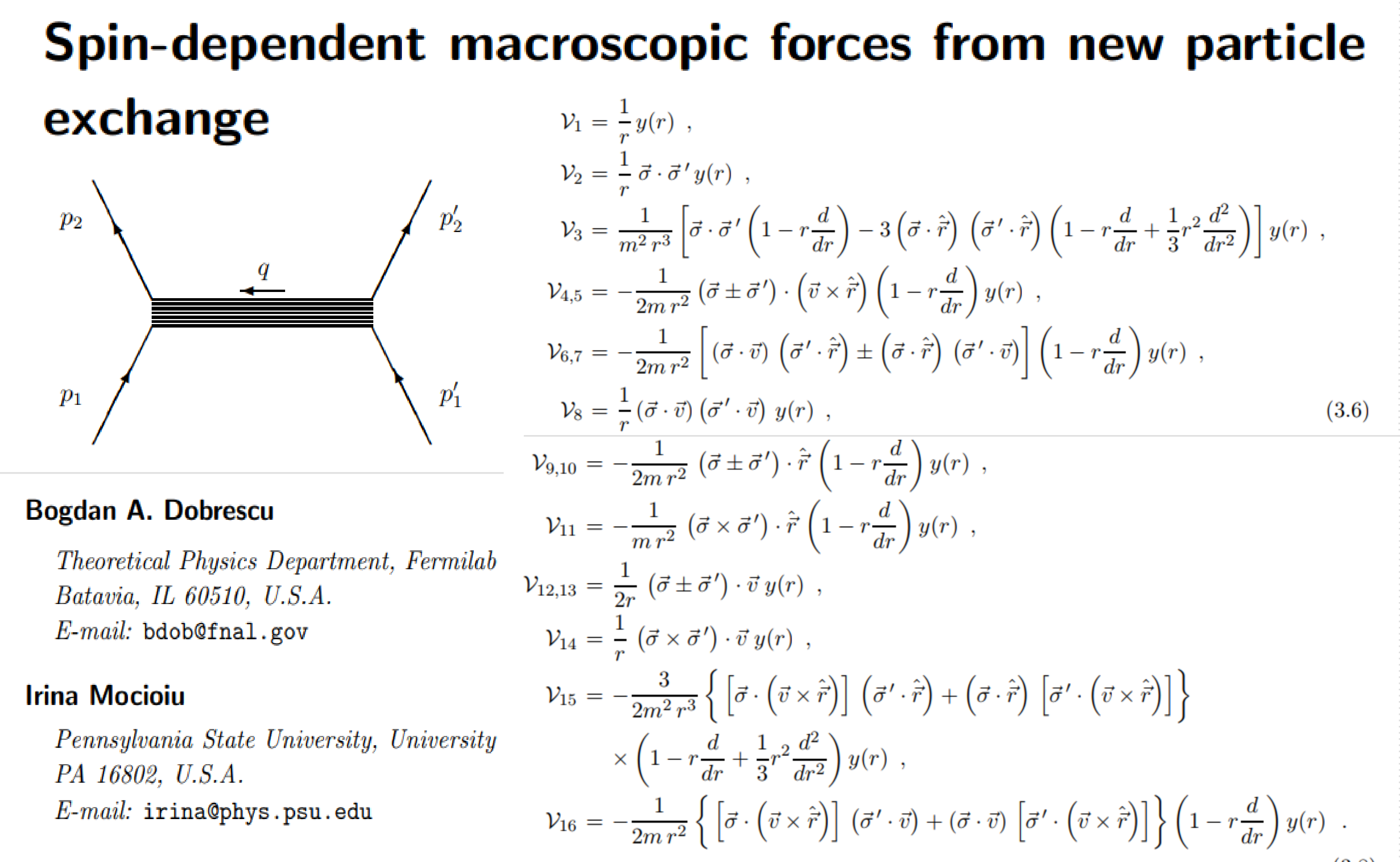
2017年《科学》杂志综述指出，除了利用耗资巨大的大型科学装置，还可以利用实验室尺度“桌面式”实验装置来研究标准模型以外的新物理。



基本原理：

- 新粒子与自旋体系相互作用
- 自旋体系本身的能级结构发生扰动（自旋感受一个等效磁场）
- 利用磁，电，光等手段精密测量能级结构的变化（利用自旋精密测磁）
- 获取未知新粒子的信息

超越标准模型的新物理探索：
十六种自旋相关的新相互作用



Spin-dependent macroscopic forces from new particle exchange

Bogdan A. Dobrescu

Theoretical Physics Department, Fermilab
Batavia, IL 60510, U.S.A.
E-mail: `bdob@fnal.gov`

Irina Mocioiu

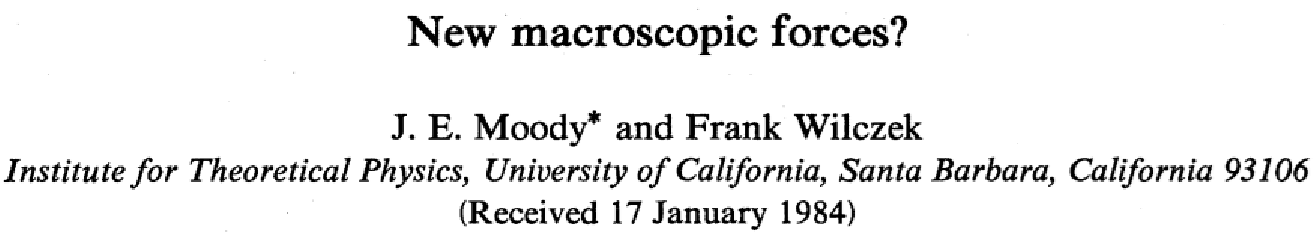
Pennsylvania State University, University
PA 16802, U.S.A.
E-mail: `irina@phys.psu.edu`

$$
\begin{aligned}
\mathcal{V}_1 &= \frac{1}{r}\, y(r) \ , \\
\mathcal{V}_2 &= \frac{1}{r}\, \vec{\sigma}\cdot\vec{\sigma}\,'\, y(r) \ , \\
\mathcal{V}_3 &= \frac{1}{m^2 r^3}\left[\vec{\sigma}\cdot\vec{\sigma}\,'\left(1 - r\frac{d}{dr}\right) - 3\left(\vec{\sigma}\cdot\hat{\vec{r}}\right)\left(\vec{\sigma}\,'\cdot\hat{\vec{r}}\right)\left(1 - r\frac{d}{dr} + \frac{1}{3}r^2\frac{d^2}{dr^2}\right)\right] y(r) \ , \\
\mathcal{V}_{4,5} &= -\frac{1}{2m\,r^2}\left(\vec{\sigma}\pm\vec{\sigma}\,'\right)\cdot\left(\vec{v}\times\hat{\vec{r}}\right)\left(1 - r\frac{d}{dr}\right) y(r) \ , \\
\mathcal{V}_{6,7} &= -\frac{1}{2m\,r^2}\left[\left(\vec{\sigma}\cdot\vec{v}\right)\left(\vec{\sigma}\,'\cdot\hat{\vec{r}}\right) \pm \left(\vec{\sigma}\cdot\hat{\vec{r}}\right)\left(\vec{\sigma}\,'\cdot\vec{v}\right)\right]\left(1 - r\frac{d}{dr}\right) y(r) \ , \\
\mathcal{V}_8 &= \frac{1}{r}\left(\vec{\sigma}\cdot\vec{v}\right)\left(\vec{\sigma}\,'\cdot\vec{v}\right) y(r) \ ,
\end{aligned}
\tag{3.6}
$$

$$
\begin{aligned}
\mathcal{V}_{9,10} &= -\frac{1}{2m\,r^2}\left(\vec{\sigma}\pm\vec{\sigma}\,'\right)\cdot\hat{\vec{r}}\left(1 - r\frac{d}{dr}\right) y(r) \ , \\
\mathcal{V}_{11} &= -\frac{1}{m\,r^2}\left(\vec{\sigma}\times\vec{\sigma}\,'\right)\cdot\hat{\vec{r}}\left(1 - r\frac{d}{dr}\right) y(r) \ , \\
\mathcal{V}_{12,13} &= \frac{1}{2r}\left(\vec{\sigma}\pm\vec{\sigma}\,'\right)\cdot\vec{v}\, y(r) \ , \\
\mathcal{V}_{14} &= \frac{1}{r}\left(\vec{\sigma}\times\vec{\sigma}\,'\right)\cdot\vec{v}\, y(r) \ , \\
\mathcal{V}_{15} &= -\frac{3}{2m^2 r^3}\left\{\left[\vec{\sigma}\cdot\left(\vec{v}\times\hat{\vec{r}}\right)\right]\left(\vec{\sigma}\,'\cdot\hat{\vec{r}}\right) + \left(\vec{\sigma}\cdot\hat{\vec{r}}\right)\left[\vec{\sigma}\,'\cdot\left(\vec{v}\times\hat{\vec{r}}\right)\right]\right\} \\
&\quad \times\left(1 - r\frac{d}{dr} + \frac{1}{3}r^2\frac{d^2}{dr^2}\right) y(r) \ , \\
\mathcal{V}_{16} &= -\frac{1}{2m\,r^2}\left\{\left[\vec{\sigma}\cdot\left(\vec{v}\times\hat{\vec{r}}\right)\right]\left(\vec{\sigma}\,'\cdot\vec{v}\right) + \left(\vec{\sigma}\cdot\vec{v}\right)\left[\vec{\sigma}\,'\cdot\left(\vec{v}\times\hat{\vec{r}}\right)\right]\right\}\left(1 - r\frac{d}{dr}\right) y(r) \ .
\end{aligned}
$$

现状与机遇

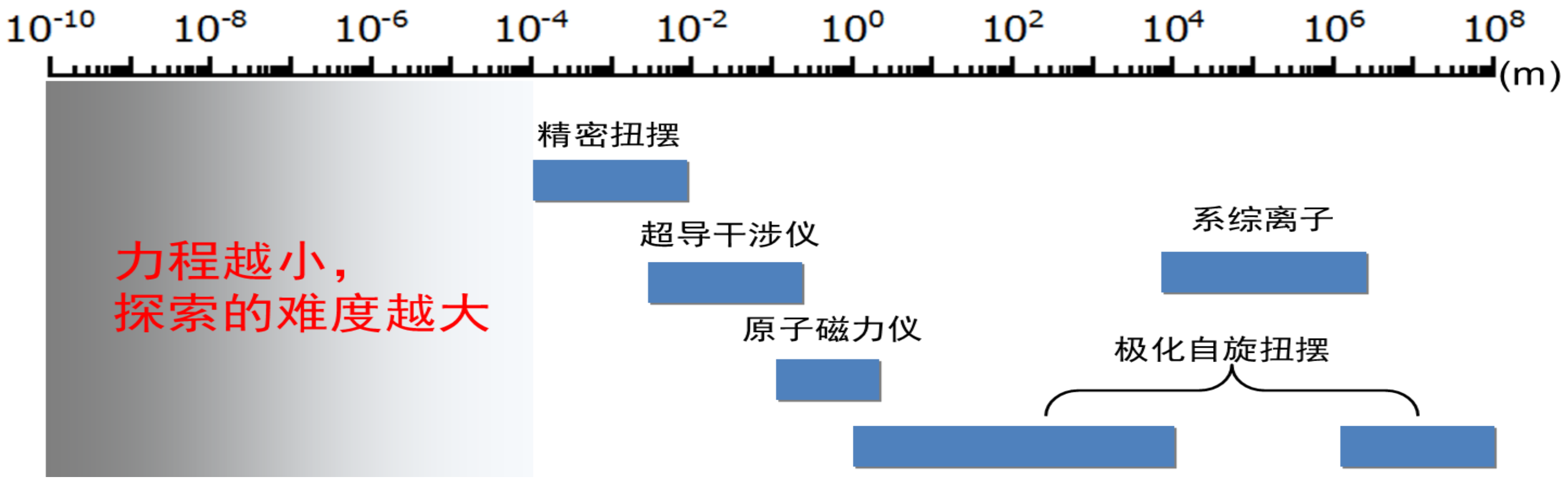
物理学诺奖获得者（2004）
Frank Wilczek



New macroscopic forces?

J. E. Moody* and Frank Wilczek
Institute for Theoretical Physics, University of California, Santa Barbara, California 93106
(Received 17 January 1984)

自旋体系可以被用来探索（类）轴子诱导的相互作用，从而为探索类轴子指出一个重要的实验方向。



现状：国际上已经在宏观尺度展开了一系列实验搜寻，目前尚未观测到。
机遇：发展新方法，打开亚毫米乃至纳米尺度探测新窗口

Searching for exotic spin-dependent interactions with NVs

- **spin-mass interaction**

$$\mathcal{V}_{9,10} = -\frac{1}{2m\,r^2}\,(\vec{\sigma} \pm \vec{\sigma}\,') \cdot \hat{\vec{r}}\,\left(1 - r\frac{d}{dr}\right) y(r) \ ,$$

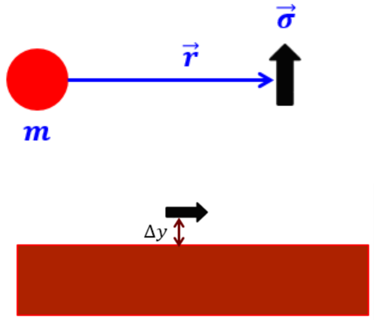
Xing Rong et al., Nature Communications 9, 739 (2018)

- **exotic dipole-dipole interaction**

$$\mathcal{V}_2 = \frac{1}{r}\,\vec{\sigma} \cdot \vec{\sigma}\,'\,y(r) \ ,$$

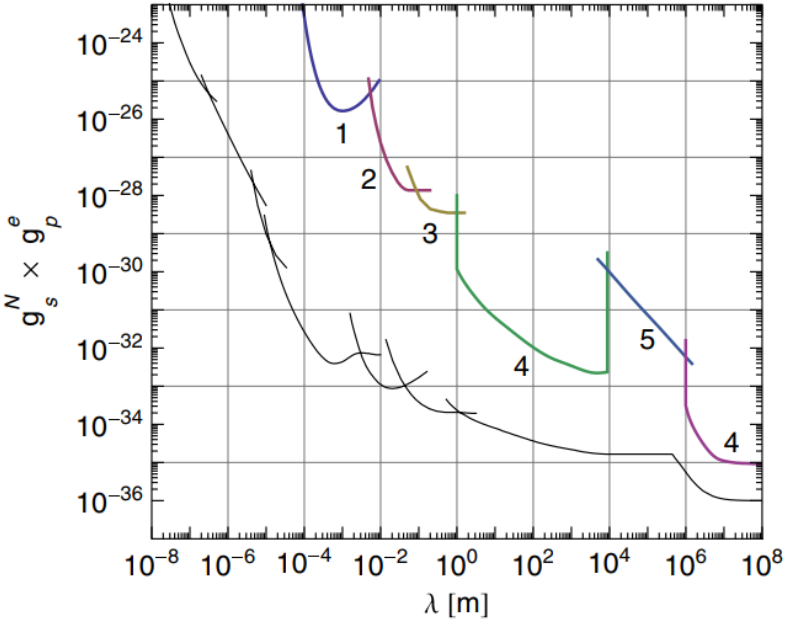
Xing Rong et al., Phys. Rev. Lett. 121, 080402 (2018)

Constraints on spin-mass interaction



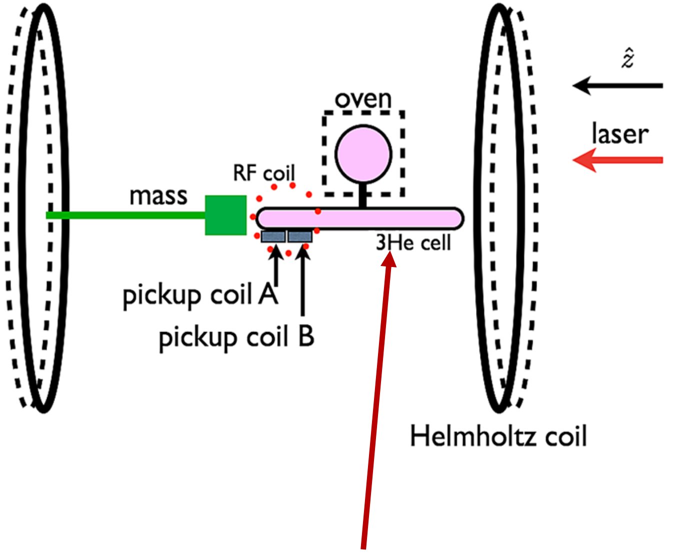
$$\vec{B}_{eff} = \frac{1}{\gamma}\frac{\hbar g_s g_p}{2m}\rho\lambda e^{-\frac{\Delta y}{\lambda}}(1-e^{-\frac{d}{\lambda}})\hat{y}$$

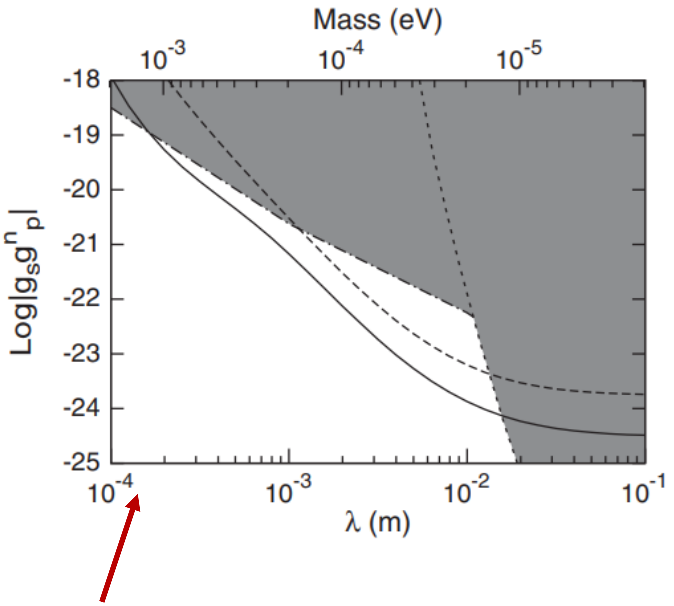
PRD 86, 015001 (2012)



One of the limitations：The size of the sensor!

Limitation of the sensor (an example)



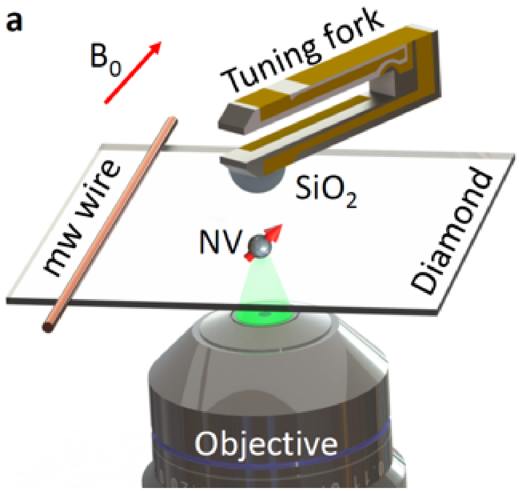


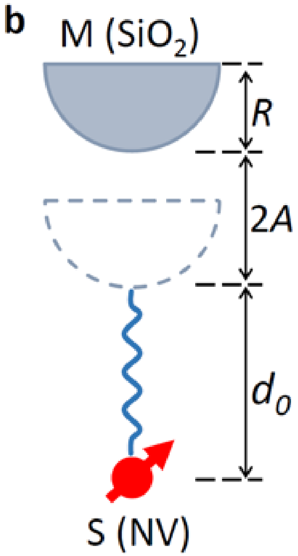
The thickness of the cell (the sensor) is 250 μm. It is very challenging to make it much thinner.

The investigated force range is above ~100 μm

PHYSICAL REVIEW D 87, 011105(R) (2013)

Constrain spin-mass interaction within μm scale





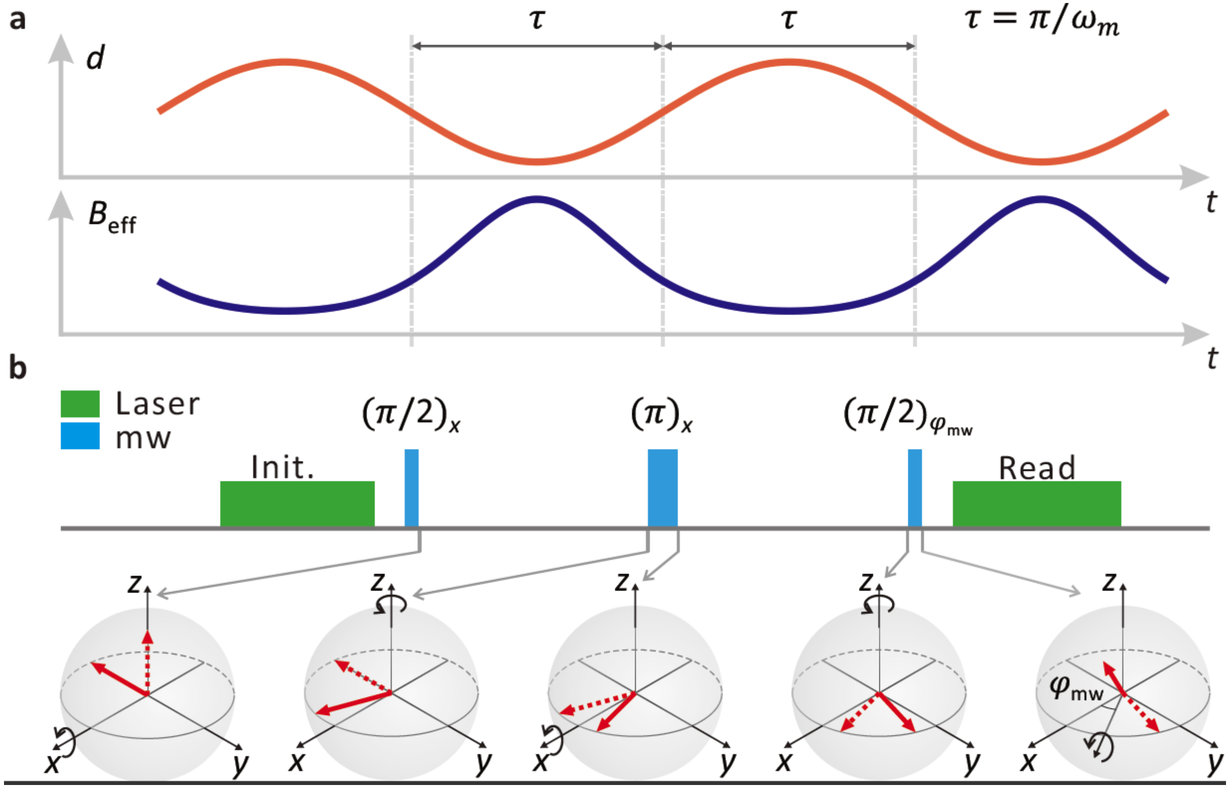
advantages

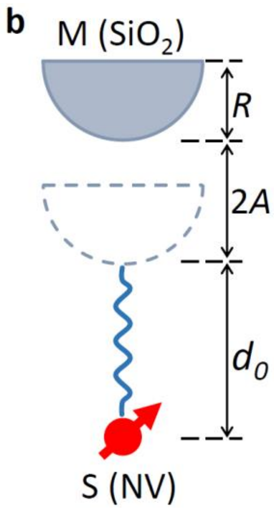
- ✓ Atomic scale
- ✓ Near surface

→ Shorter force range

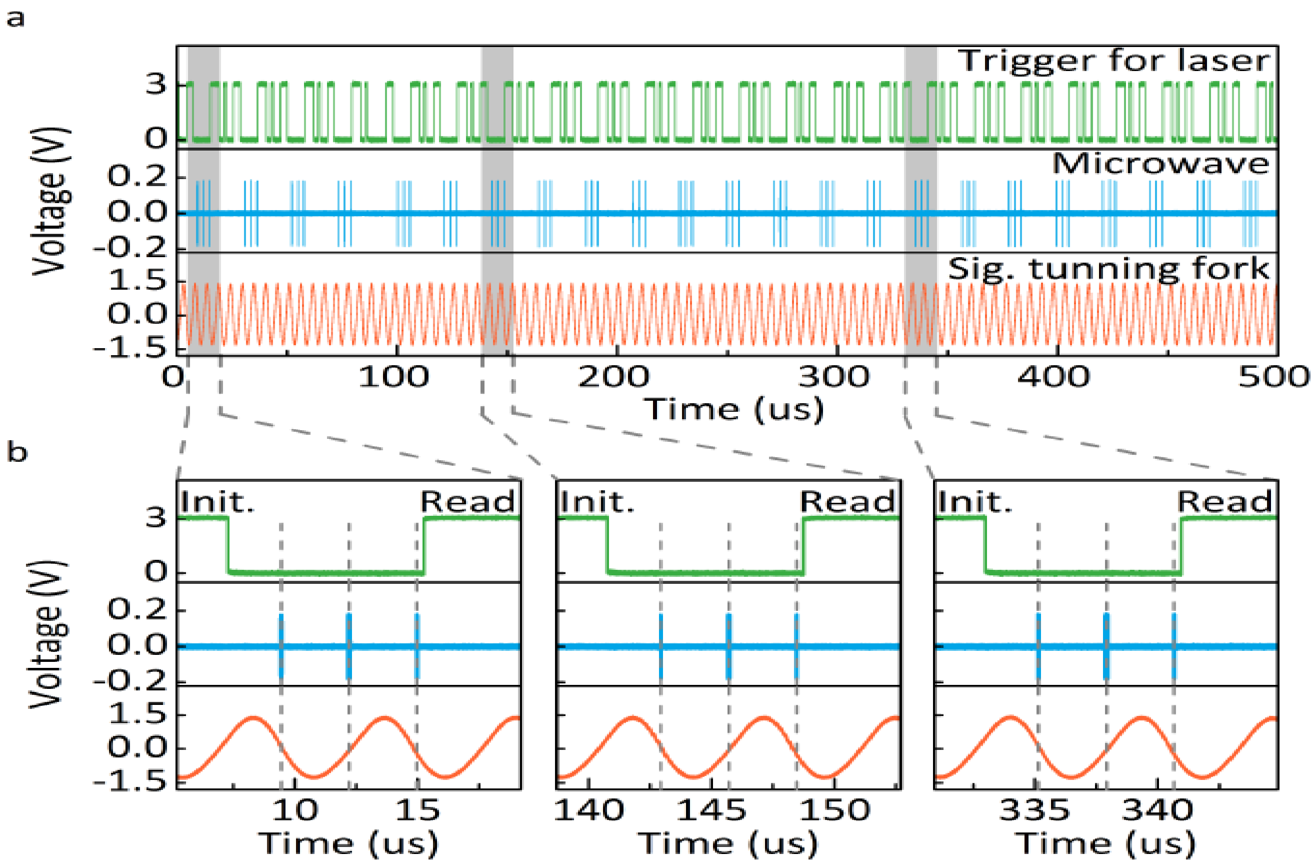
- ✓ Precise quantum control → Good sensitivity
- ✓ NV + AFM → Cancel unwanted signals

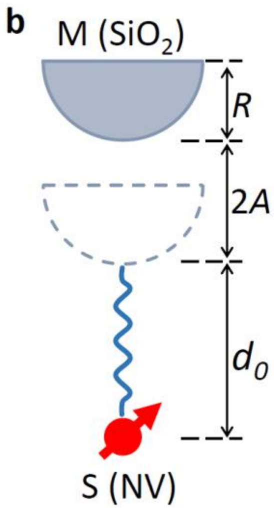
Encoding the hypothetical magnetic field in the state of NV



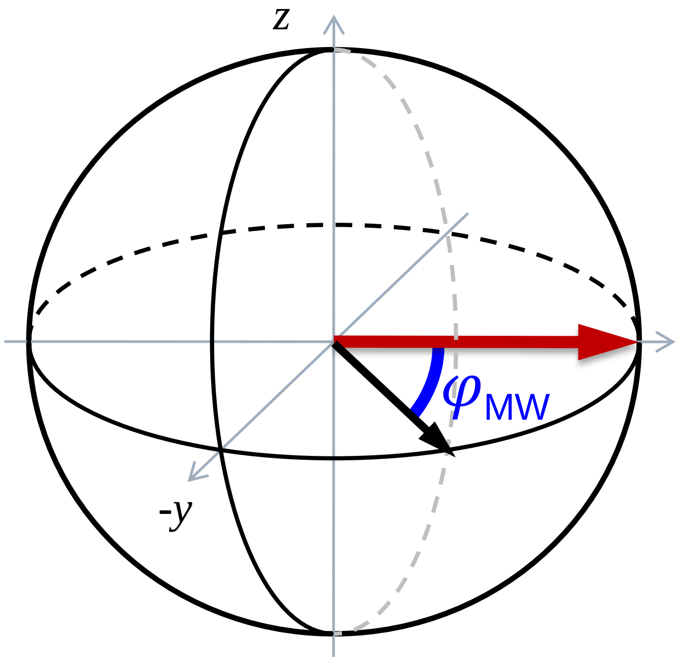


Experimental time sequence

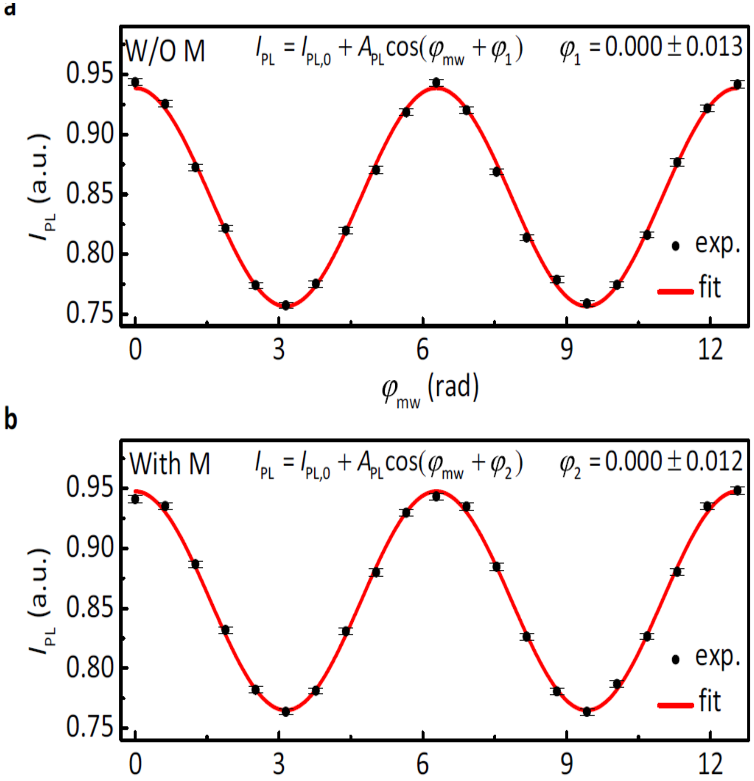




Experimental result

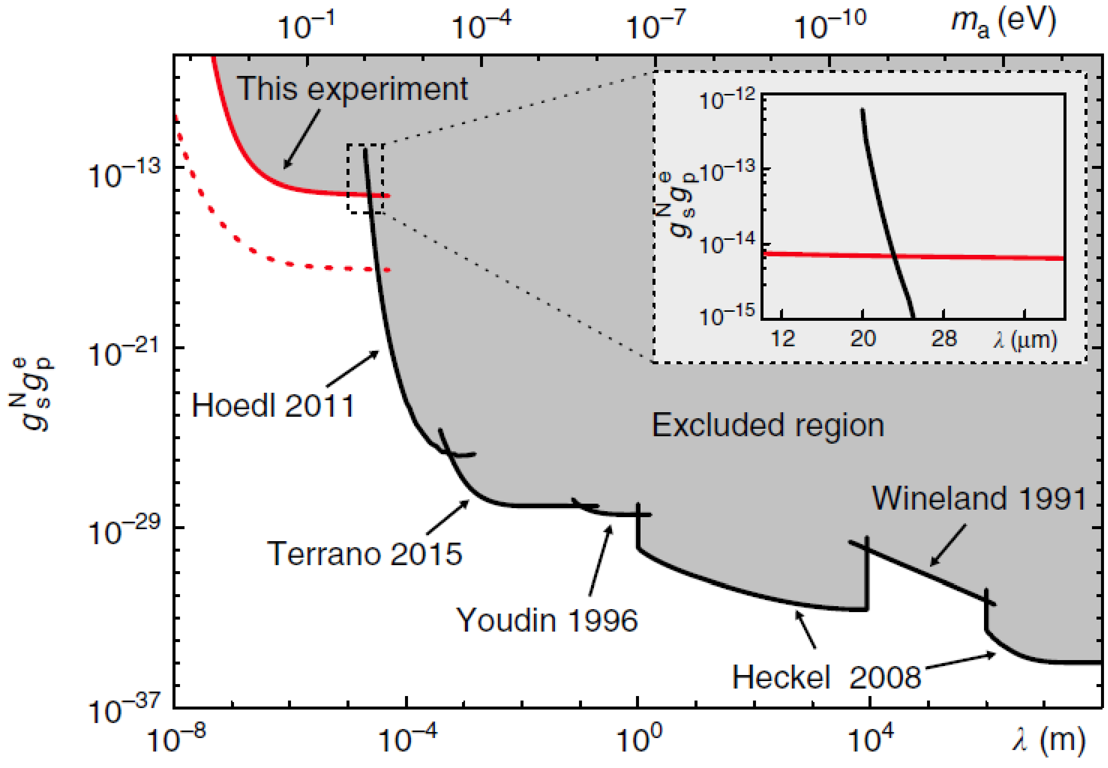


Changing the phase of last microwave pulse: φ_{MW}

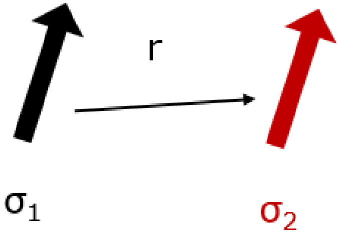


statistical errors: ～ 0.018 rad

Constraints by our experiment



Constraint on exotic interaction between electrons



Magnetic dipole-dipole coupling

$$-\frac{\mu_0\gamma_e\gamma_e\hbar^2}{16\pi r^3}[3(\vec{\sigma_1}\cdot\hat{r})(\vec{\sigma_2}\cdot\hat{r})-(\vec{\sigma_1}\cdot\vec{\sigma_2})],$$

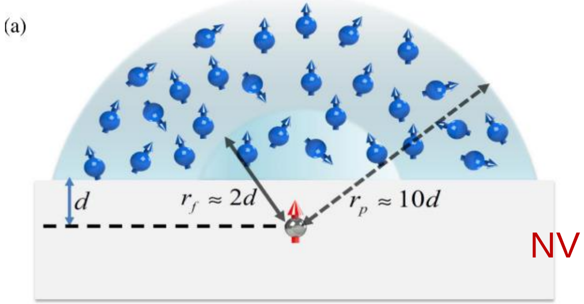
Exotic dipole-dipole coupling [1]

$$\frac{g_A^e g_A^e}{4\pi\hbar c}\frac{\hbar c}{r}(\vec{\sigma_1}\cdot\vec{\sigma_2})e^{-\frac{r}{\lambda}},$$

We now experimentally search for this type of exotic dipole-dipole coupling [2, 3].

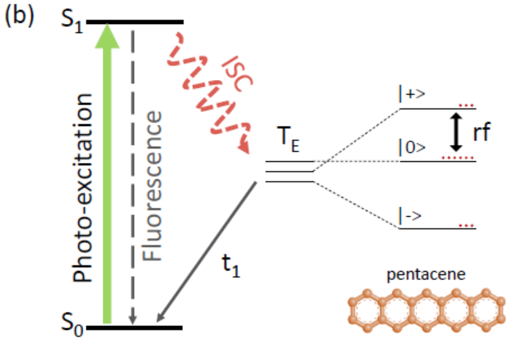
[1] B. A. Dobrescu and I.Mocioiu, J. High Energy Phys. 11, 005 (2006)
[2] Xing Rong et al., Phys. Rev. Lett. 121, 080402 (2018)

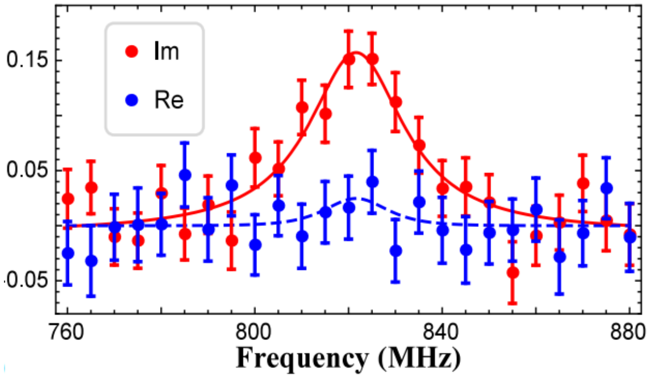
Experiment method



pentacene

NV in diamond





- Imaginary: polarized signal

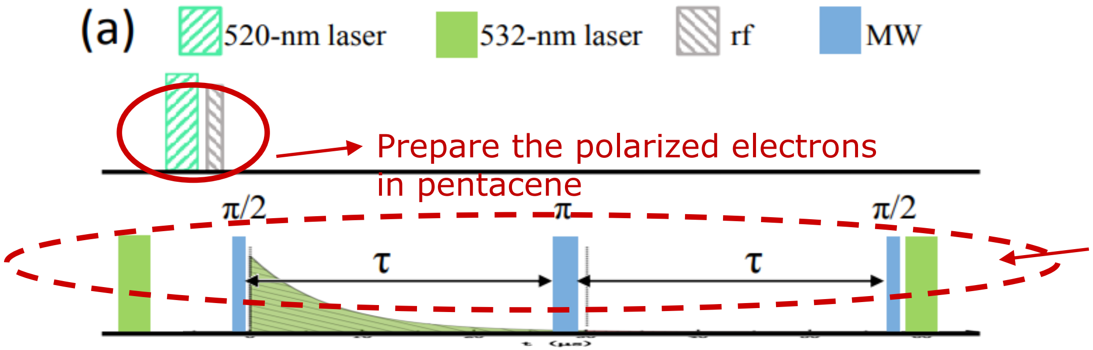
$$\bar{B} = \frac{\mu_0 g_s}{6} M = \frac{4\pi c\rho P}{3},$$

- Real: fluctuation signal

$$(\delta B)^2 = \frac{\pi c^2 \rho (1 - P^2)}{4d^3} \doteq \frac{\pi c^2 \rho}{4d^3},$$

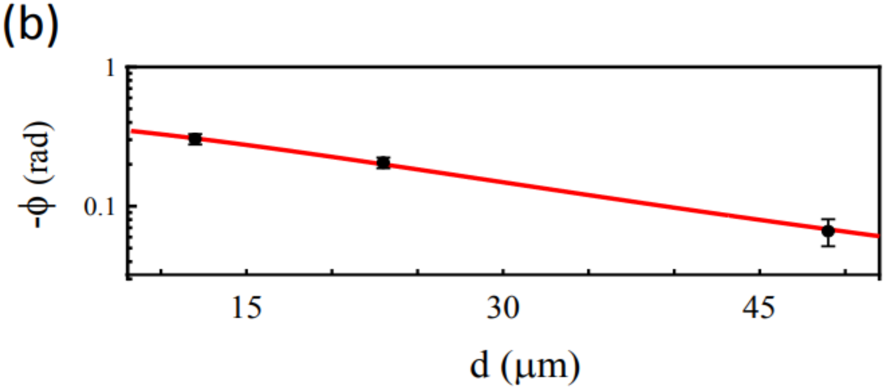
T. Xie et al., Phys. Rev. Applied 9, 064003 (2018).

Experimental pulse sequence



Prepare the polarized electrons in pentacene

Detect polarized signal by NV

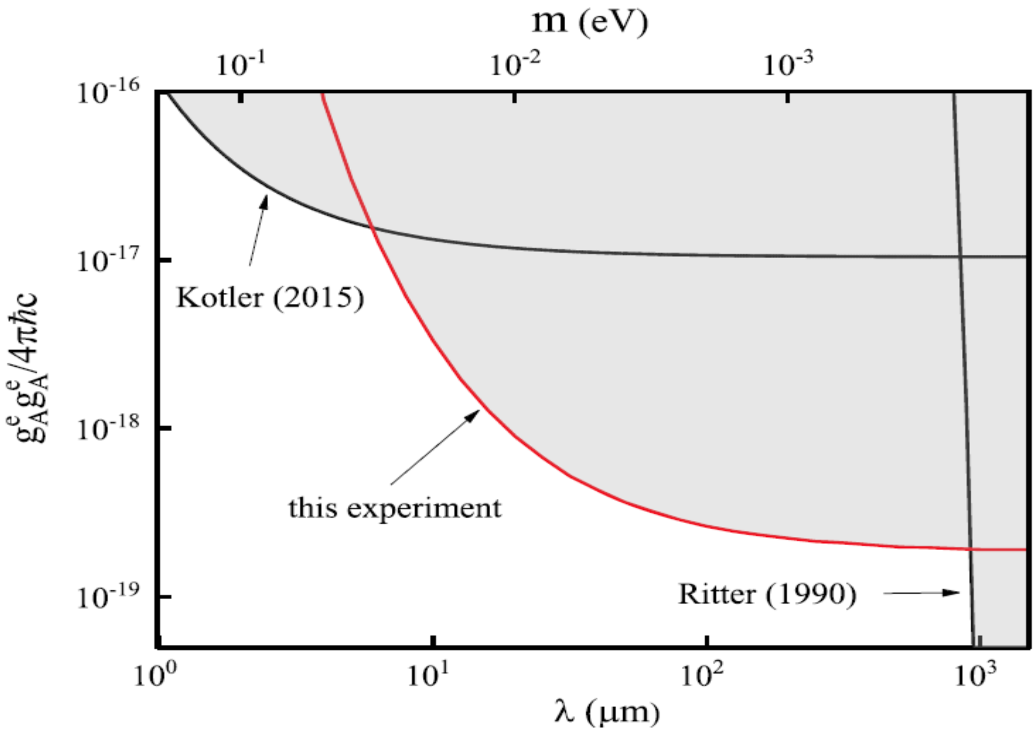


Fitting to the experiment data with both of the two interactions included

$$\frac{g_A^e g_A^e}{4\pi\hbar c} = (-0.78 \pm 1.46) \times 10^{-20}$$

Xing Rong et al., Phys. Rev. Lett. 121, 080402 (2018)

New constraint on exotic interaction between electrons



We established upper limits on this type of exotic spin-dependent interaction in the force range 10 to 900 μm.

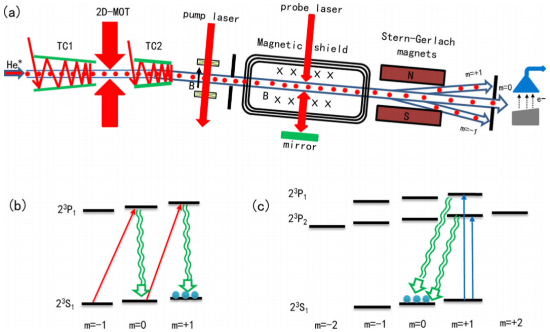
Xing Rong et al., Phys. Rev. Lett. 121, 080402 (2018)

学术评价和影响

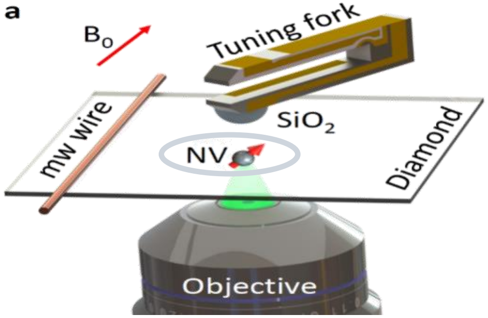
Dmitry Budker 于2018年8月发表综述，总结了四大类实验室尺度探索（类）轴子诱导新奇相互作用的方法。文中指出：基于NV色心 量子传感器方法是由科大杜团队提出并实验实现。

Ann. Phys. (Berlin) 531,1800273 (2019)

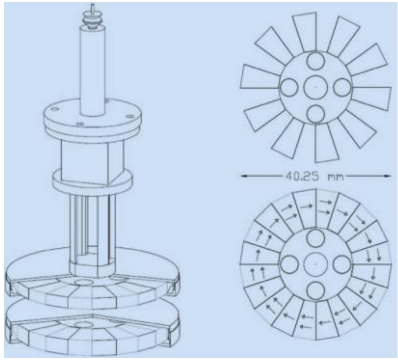
原子光谱 (10^{-10} -10^{-9} m)



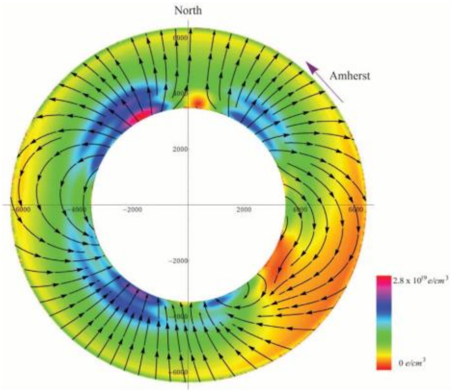
金刚石NV色心(10^{-9} -10^{-3} m)



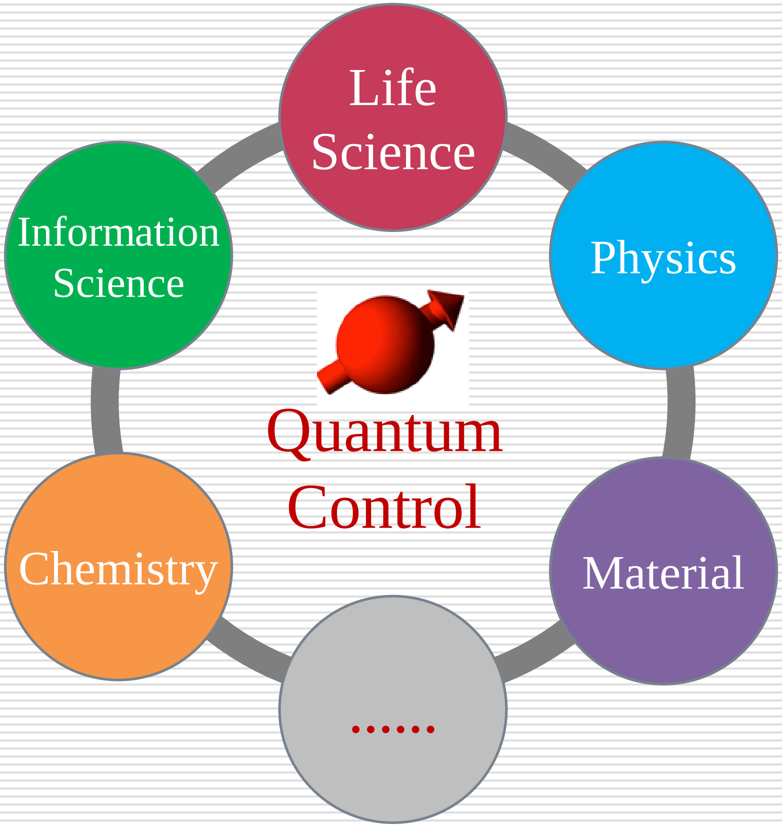
精密扭秤(10^{-3} -10-1 m)



地质电子(10^{-1} -10^{8} m)



Summary



Life Science

Physics

Material

……

Chemistry

Information Science

Quantum Control

- ➢ Spin is among the most promising physical systems for quantum control.
- ➢ Spin holds the promise of realizing various novel quantum applications.

A particular application in the foreseeable future:

Single-molecule MR Spectroscopy and Imaging

Acknowledge

My group members

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Hope for collaborations with you!

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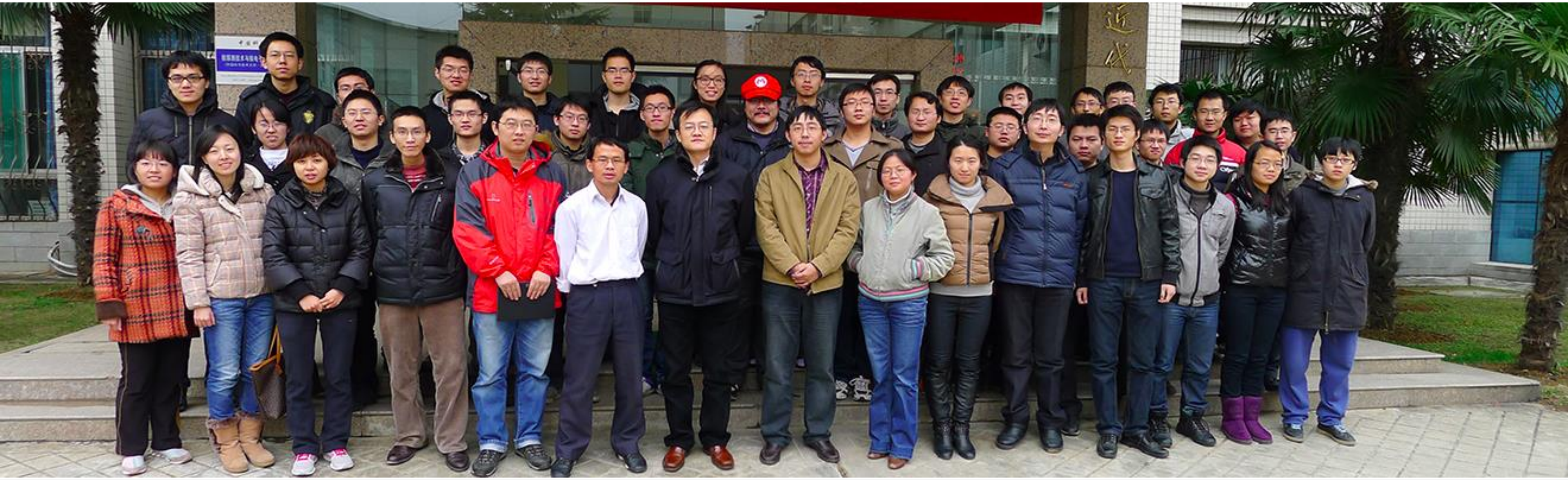
Thanks for your attention



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