MOLECULAR MAGNETS FOR QUANTUM COMPUTING - EXPERIMENTAL PERSPECTIVES

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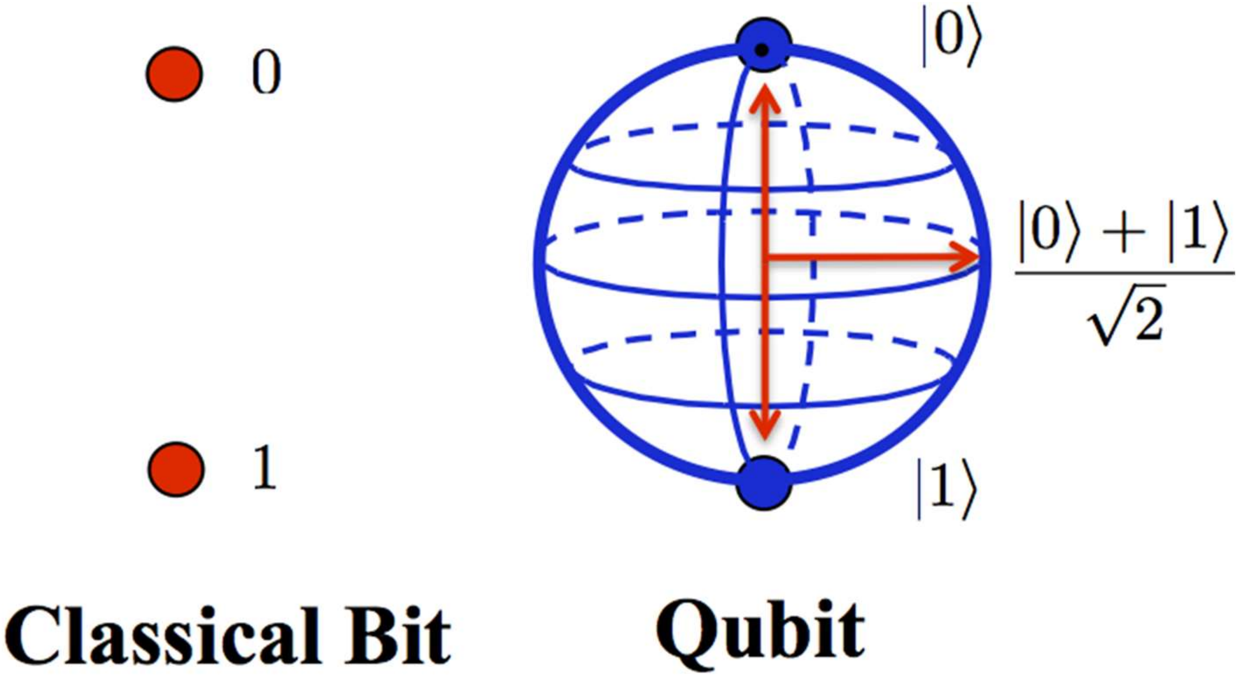
The Plan

- *Quantum bits, quantum gates, Bloch sphere, decoherence*
- *Magnetic resonance as a tool for quantum computing*
- *Mononuclear magnetic molecules & spin clusters as qubits*
- *Soliton qubits*
- *Quantum entanglement in low-dimensional magnets*

Quantum bits

- *qubit* – two-state quantum object, can be in the state of superposition $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$
  - for probability of states $|\alpha|^2 + |\beta|^2 = 1$



Quantum bits

Important requirements (DiVicenzo criteria)

- Well-defined objects
  - Addressability, possibility to create exact spatial structures of qubits
- Initialization of qubit, defined initial state
  - polarizer
- Long enough quantum coherence time in comparison with quantum gate operation time = qubit figure of merit
  - decoherence, Rabi oscillations
- Universal set of quantum gates (minimálna úplná množina log. hradiel)
  - gates NOT a CNOT
- Possibility to measure resulting state
  - Result of quantum computation

Quantum bits = spins

Important requirements (DiVicenzo criteria)

- Well-defined objects
  - Electron or nuclear spin, etc.
- Initialization of qubit, defined starting state
  - Static magnetic field, electric field
- Long enough quantum coherence time in comparison with quantum gate operation time = qubit figure of merit
  - Experimentally observed on el. spins < 1 ms at liquid nitrogen temperatures
- Universal set of quantum gates (minimálna úplná množina log. hradiel)
  - Short pulse of magnetic field or series of timed pulses
- Possibility to measure resulting state
  - Detection coil, spin-polarized STM

Quantum bits = electron spins

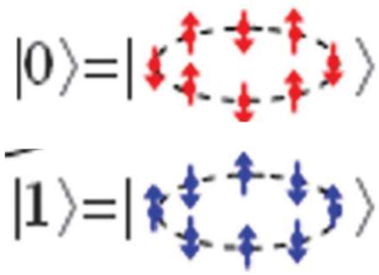
- *Definition of qubit – electron spin !*

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$|0\rangle = |S = 1/2, m_s = -1/2\rangle$$

$$|1\rangle = |S = 1/2, m_s = 1/2\rangle$$

- magnetic defects (NV center in diamond), molecules with 3d or 4f ion, spin cluster with well defined ground state with S=1/2



- topological objects with well defined quantum states – solitons in one-dimensional magnets
- *Preparation of initial qubit state* – static magnetic field selects one state, e.g. $|0\rangle$

Quantum gate

- *We can perform arbitrary unitary transformation*

$$\left|\psi(t)\right\rangle = U\left|\psi(0)\right\rangle$$

  - Later we show how to perform it on spin

- *Set of simple qubit logic gates*

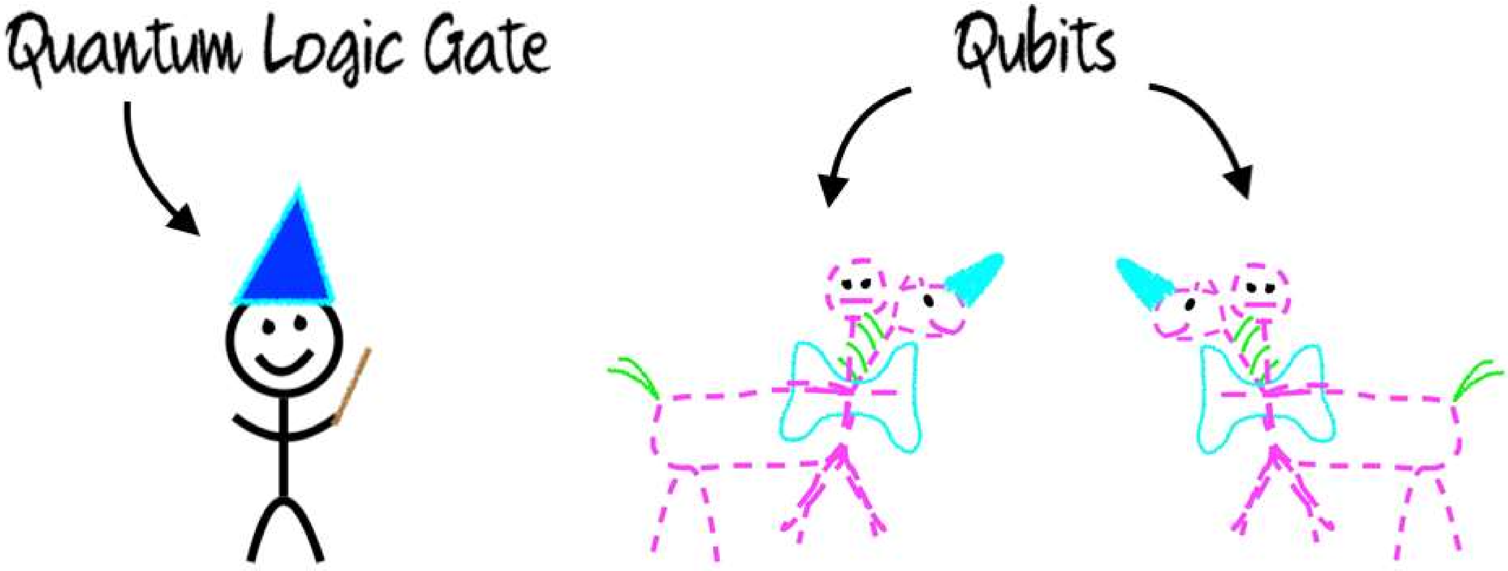
		truth table
$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	Unity	$\alpha\|0\rangle + \beta\|1\rangle \xrightarrow{I} \alpha\|0\rangle + \beta\|1\rangle$
$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	NOT	$\alpha\|0\rangle + \beta\|1\rangle \xrightarrow{X} \beta\|0\rangle + \alpha\|1\rangle$
$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$	Phase	$\alpha\|0\rangle + \beta\|1\rangle \xrightarrow{S} \alpha\|0\rangle + i\beta\|1\rangle$
$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	Hadamard	$\alpha\|0\rangle + \beta\|1\rangle \xrightarrow{H} \alpha\frac{\|0\rangle + \|1\rangle}{\sqrt{2}} + \beta\frac{\|0\rangle + \|1\rangle}{\sqrt{2}}$

Quantum gate

- *We can perform arbitrary unitary transformation*

$$|\psi(t)\rangle = U|\psi(0)\rangle$$

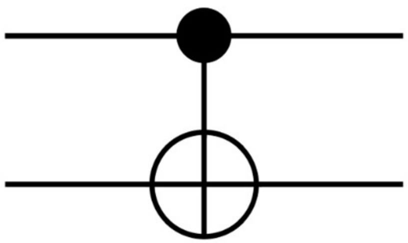
Fairicorn qubit



Quantum gate

- *Universal set of quantum gates (minimálna úplná množina) allows to perform all possible logic operations – e.g. NOT and CNOT*
  - NOT – one-qubit gate - spin-flip – preklopenie spinu

  - CNOT (controlled-NOT or XOR) – two-qubit gate – requires the possibility to switch off and on interaction between qubits, changing first qubit state using quantum entanglement we change the second qubit state, but only if control qubit is $|1\rangle$



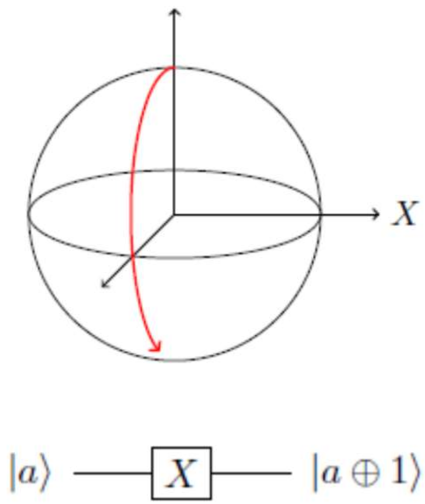
Starting state		Ending State
|00>	→	|00>
|10>	→	|10>
|01>	→	|11>
|11>	→	|01>

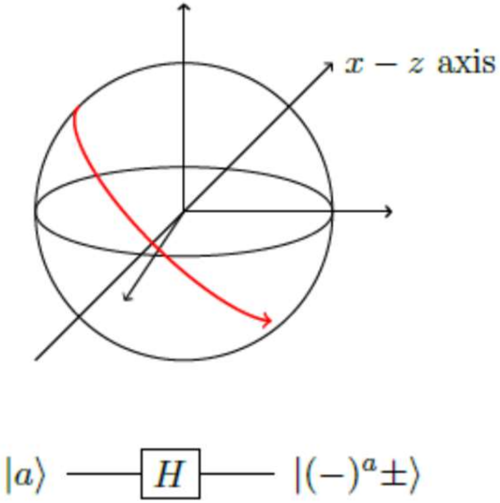
Bloch sphere

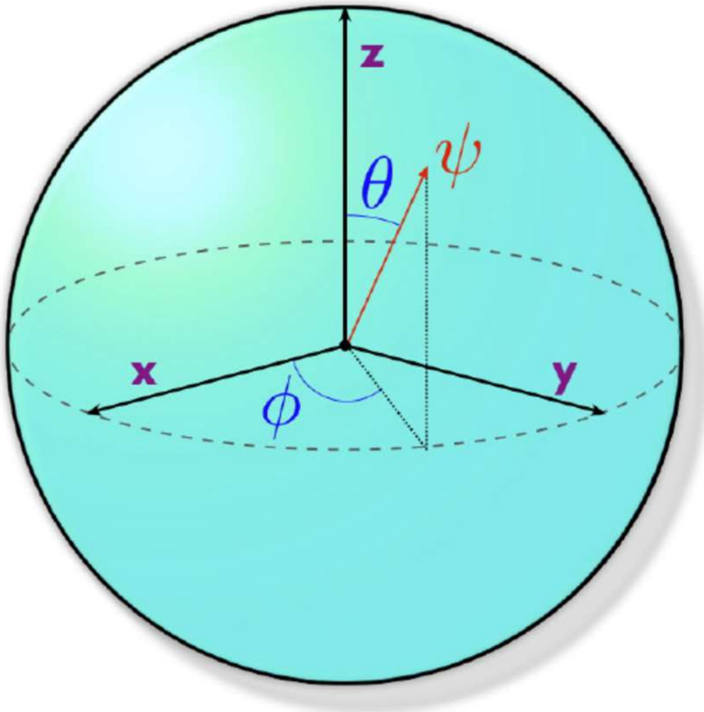
- *Bloch sphere* – description of qubit state using a vector, vector defines a point on Bloch sphere, description of quantum gates

Using polar coordinates

$$|\Psi\rangle = cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi} sin\left(\frac{\theta}{2}\right)|1\rangle$$







Bloch sphere

- *Density matrix* – defined using propability p_i that qubit is in pure state $|\Psi_i\rangle$, 2-by-2 matrix for 2-state system

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix} 1+\cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & 1-\cos\theta \end{pmatrix} = \frac{1}{2}(I + x\sigma_x + y\sigma_y + z\sigma_z)$$

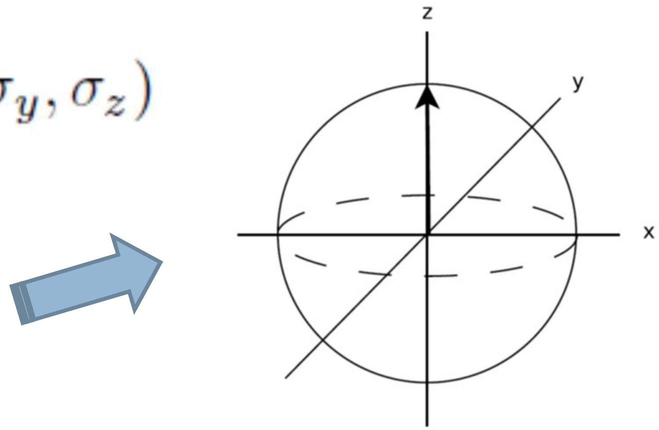
- Components of Bloch vector (*x,y,z*) define the state of qubit

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli matrices

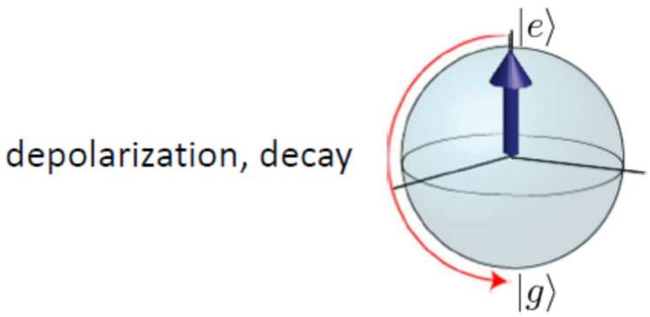
$$\rho = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma}), \quad \vec{r} = (x, y, z), \quad \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

e.g. vector (0,0,1) represents pure state $|0\rangle$



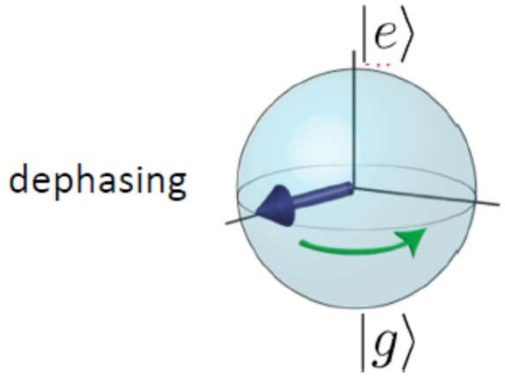
Decoherence

- The loss of quantum information due to the interaction of qubit with environment, even with other qubits



population relaxation time T_1 – lifetime of classical bit, result of the energy exchange with environment, e.g. lattice, after quantum gate operation the spin returns to equilibrium initial state (spin-lattice relaxation time),

- this is upper limit for T_2



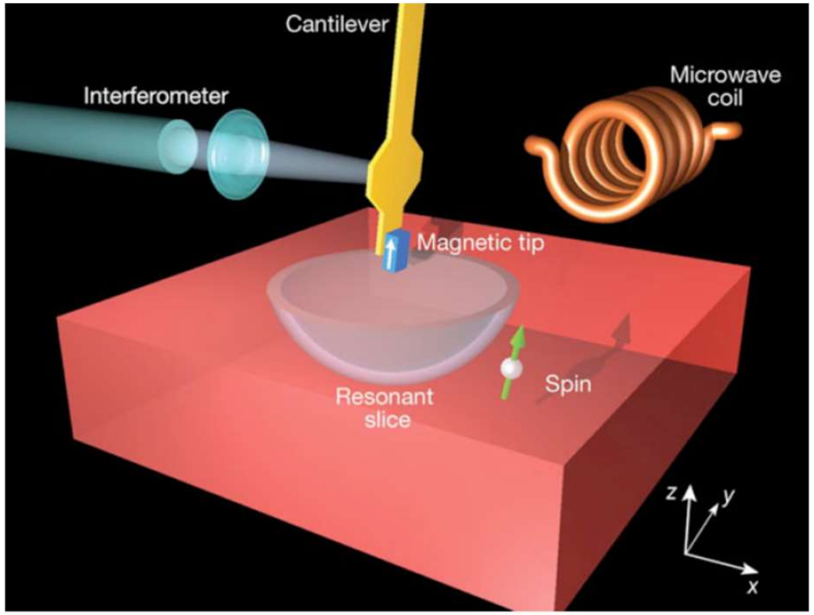
phase memory time T_2 – lifetime of quantum bit encoded in the phase of quantum state – interaction with other qubits – mutual interaction between electron spins or electron-nuclear (hyperfine) interaction, the measurement itself leads to decoherence (spin-spin relaxation time)

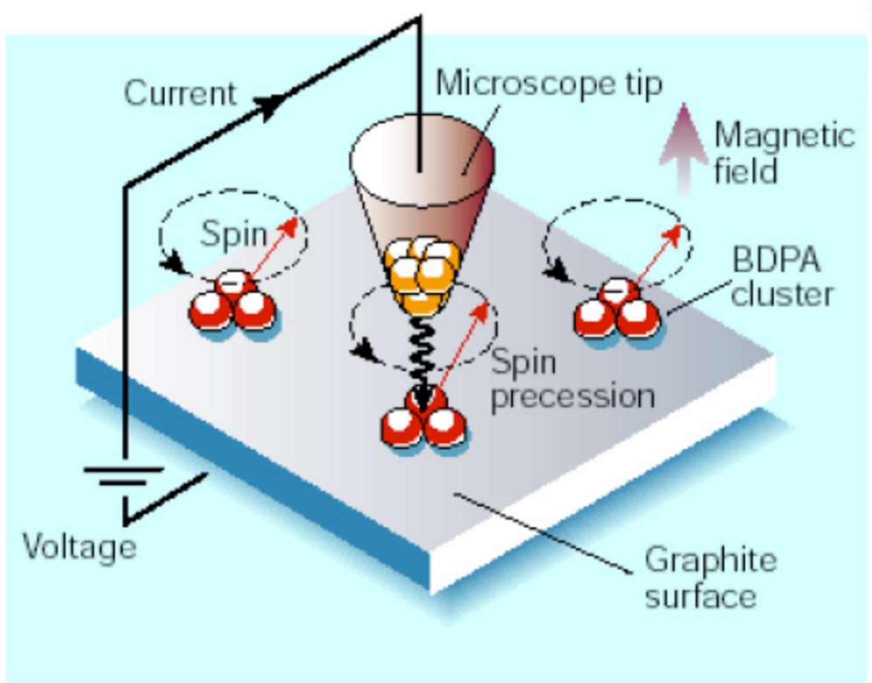
Decoherence

- Qubit figure of merit – ratio of quantum coherence time (period when quantum information is preserved) and quantum gate operation time – needs to be in order of 10^4
- Technologically obtainable quantum gate operation is about 10-20 ns → minimum quantum coherence time needs to be 100 μs (experiments exist!)

Qubit vs. Qubit Ensemble

- Ultimate goal is to have spatial arrangement of qubits (single molecules or spins), manipulate the qubit state, perform quantum gate, switch on interaction – entangle selected qubits and read the result of computation from each qubit





Qubit vs. Qubit Ensemble

- So far we don't know manipulate single spins and read their state very well - *can we study bulk sample with the aim to find whether the molecules in the sample are plausible tool for quantum computing?*
- for single qubit we can create superposition of states – *can we create an effective pure quantum state in an ensemble of qubits, perform quantum gate and then obtain the same result as we were working with single qubit?*
- *YES !*

Science AAAS

Bulk Spin-Resonance Quantum Computation
Neil A. Gershenfeld and Isaac L. Chuang
Science **275**, 350 (1997);
DOI: 10.1126/science.275.5298.350

PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

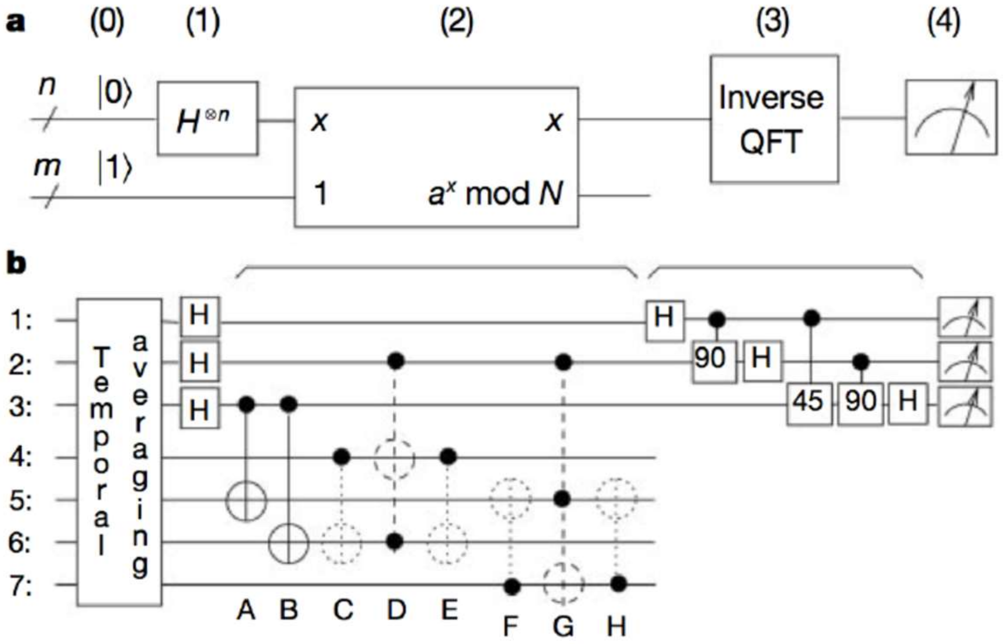
Bulk quantum computation with nuclear magnetic resonance: theory and experiment

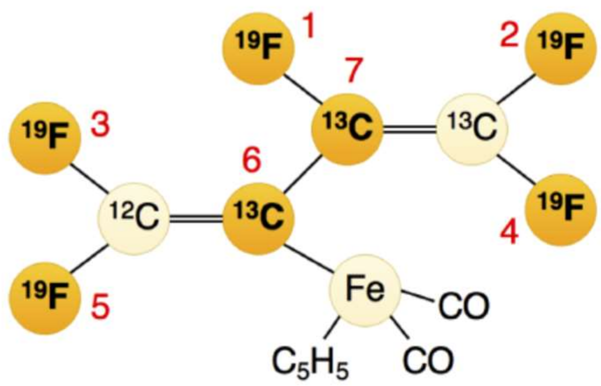
I. L. Chuang, N. Gershenfeld, M. G. Kubinec and D. W. Leung

Proc. R. Soc. Lond. A 1998 **454**, 447-467
doi: 10.1098/rspa.1998.0170

Qubit vs. Qubit ensemble

- Possibility to encode some of quantum algorithms in several different states of one molecule or different spins in molecule – Shor algorithm for factorization of large numbers using NMR on different nuclei in the molecule (factorization of N = 15)





Magnetic resonance

- Interaction of vector $\vec{r}$ with vector $\vec{B}$ so that its magnitude is not altered - interaction of magnetic moment with magn. field

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r} = \frac{2\mu}{\hbar}\boldsymbol{r} \times \boldsymbol{B}$$

- Length of vector $\vec{r}$ is preserved, pure quantum state of qubit is preserved also

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{r} \cdot \boldsymbol{r}) = 2\boldsymbol{r} \cdot \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r} = \frac{4\mu}{\hbar}\boldsymbol{r} \cdot (\boldsymbol{r} \times \boldsymbol{B}) = 0$$

- Let the field be static and uniform

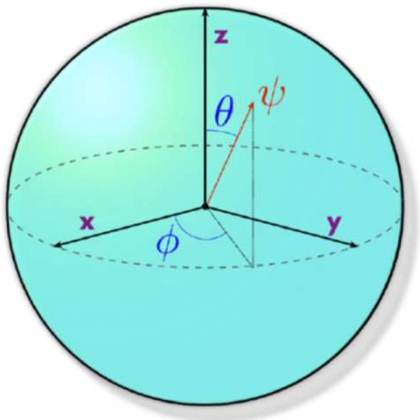
in the *z* direction→ $\boldsymbol{B} = B\boldsymbol{e}_z$

$$\begin{aligned} \frac{\mathrm{d}r^x}{\mathrm{d}t} &= \frac{2\mu}{\hbar} r^y B, \\ \frac{\mathrm{d}r^y}{\mathrm{d}t} &= -\frac{2\mu}{\hbar} r^x B \\ \frac{\mathrm{d}r^z}{\mathrm{d}t} &= 0. \end{aligned}$$

Magnetic resonance

- vector $\vec{r}$ rewritten using polar coordinates on Bloch sphere

$$r = \begin{pmatrix} \cos\phi(t)\sin\theta(t) \\ \pm\sin\phi(t)\sin\theta(t) \\ \cos\theta(t) \end{pmatrix}$$



- Solve differential equation

$$\frac{\mathrm{d}r^z}{\mathrm{d}t} = 0$$

→ θ does not change

→ the probability of finding the qubit in state $|1\rangle$ alebo $|0\rangle$ does not change

$$\frac{\mathrm{d}r^x}{\mathrm{d}t} = \frac{2\mu}{\hbar} r^y B, \qquad \frac{\mathrm{d}r^y}{\mathrm{d}t} = -\frac{2\mu}{\hbar} r^x B$$

$$r^x(t) = r_0^x \cos\omega_L t$$

$$r^y = \frac{1}{\omega_L}\frac{\mathrm{d}}{\mathrm{d}t} r^x = -\frac{1}{\omega_L}\omega_L r_0^x \sin\omega_L t = -r_0^x \sin\omega_L t$$

- Similar to harmonic oscillator

Magnetic resonance

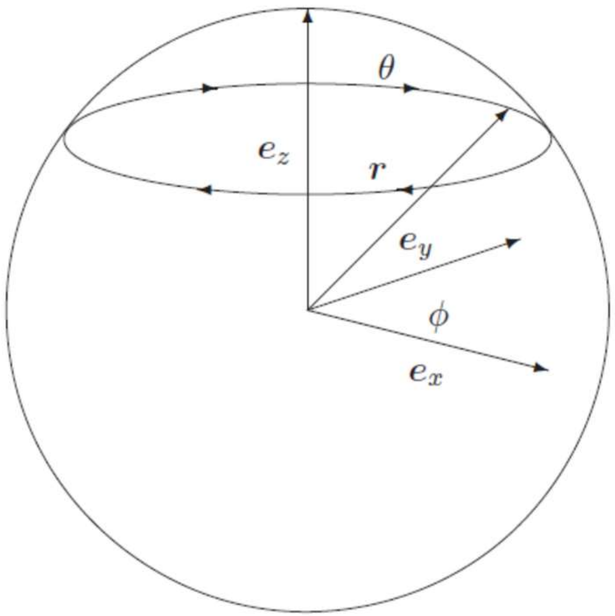
- Larmor frequency

$$\phi(t) = \omega_L t$$

$$\omega_L = \frac{2\mu B}{\hbar}$$

$$\begin{aligned} r^x &= \sin\theta\cos\omega_L t, \\ r^y &= -\sin\theta\sin\omega_L t. \\ r^z &= \cos\theta. \end{aligned}$$

Solution – vector $\vec{r}$ rotates around the magnetic field vector (precession) and his projection in the field axis remains constant



Magnetic resonance

- Larmor frequency

$$
\begin{aligned}
r^x &= \sin\theta\cos\omega_L t, \\
r^y &= -\sin\theta\sin\omega_L t. \\
r^z &= \cos\theta.
\end{aligned}
$$

Probability of finding qubit in the state $|1\rangle$ or $|0\rangle$ is constant at the precession

! But, probability of finding qubit in the state of superposition

$|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is changing in time $\frac{1}{2}(1+\sin\theta\cos\omega_L t)$

Magnetic resonance

- How to change the state from $|0\rangle$ to $|1\rangle$?

Let's apply small alternating field in the plane perpendicular to static field axis *z* :

$$\begin{aligned} |B^x| &\ll |B^z|, \\ |B^y| &\ll |B^z|, \\ B^z &= \text{const.} \end{aligned}$$

$$\begin{aligned} \frac{\mathrm{d}r^x}{\mathrm{d}t} &= \frac{2\mu}{\hbar}(r^y B^z - r^z B^y) \\ \frac{\mathrm{d}r^y}{\mathrm{d}t} &= \frac{2\mu}{\hbar}(r^z B^x - r^x B^z) \\ \frac{\mathrm{d}r^z}{\mathrm{d}t} &= \frac{2\mu}{\hbar}(r^x B^y - r^y B^x) \end{aligned}$$

Solution is proposed in the from

$$\begin{aligned} r^x &= \sin\theta(t)\cos\omega_L t, \\ r^y &= -\sin\theta(t)\sin\omega_L t, \\ r^z &= \cos\theta(t). \end{aligned}$$

- We expect to find a precession around *z*, but the angle θ varies in time, much slower than the angle ϕ

Magnetic resonance

- We expect to find a precession around *z*, but the angle θ varies in time, much slower than the angle ϕ, we can neglect some terms

$$\frac{\mathrm{d}r^x}{\mathrm{d}t} = \frac{2\mu}{\hbar}\left(r^y B^z - r^z B^y\right)$$
$$\frac{\mathrm{d}r^y}{\mathrm{d}t} = \frac{2\mu}{\hbar}\left(r^z B^x - r^x B^z\right)$$
$$\frac{\mathrm{d}r^z}{\mathrm{d}t} = \frac{2\mu}{\hbar}\left(r^x B^y - r^y B^x\right)$$

$\Rightarrow$

$$\frac{\mathrm{d}r^x}{\mathrm{d}t} = \frac{2\mu}{\hbar} r^y B,$$
$$\frac{\mathrm{d}r^y}{\mathrm{d}t} = -\frac{2\mu}{\hbar} r^x B$$

we need to solve only the last equation

$$\frac{\mathrm{d}}{\mathrm{d}t} r^z = \frac{\mathrm{d}}{\mathrm{d}t}\cos\theta(t) = -\sin\theta(t)\frac{\mathrm{d}}{\mathrm{d}t}\theta(t) = \frac{2\mu}{\hbar}\left(B^y \sin\theta(t)\cos\omega_L t + B^x \sin\theta(t)\sin\omega_L t\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta(t) = \frac{2\mu}{\hbar}\left(B^x \sin\omega_L t + B^y \cos\omega_L t\right)$$

Magnetic resonance

- Let's define perpendicular alternating field and $B^z \equiv B_\parallel$

$$B^x = B_\perp \sin \omega t, \quad B^y = B_\perp \cos \omega t. \quad \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\theta(t) = \frac{2\mu B_\perp}{\hbar}\left(\sin \omega_L t \sin \omega t + \cos \omega_L t \cos \omega t\right)$$

- Assuming precession around *z*, but the angle θ is time dependent

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta(t) = \frac{2\mu B_\perp}{\hbar}\cos\left(\omega_L - \omega\right) t$$

If at t = 0 qubit is in the stat e$|0\rangle$ $\Rightarrow$ $\theta(t) = \frac{2\mu B_\perp}{\hbar}\frac{\sin\left(\omega_L - \omega\right) t}{\omega_L - \omega}$

→ Find the solution in the resonance $\omega = \omega_L$

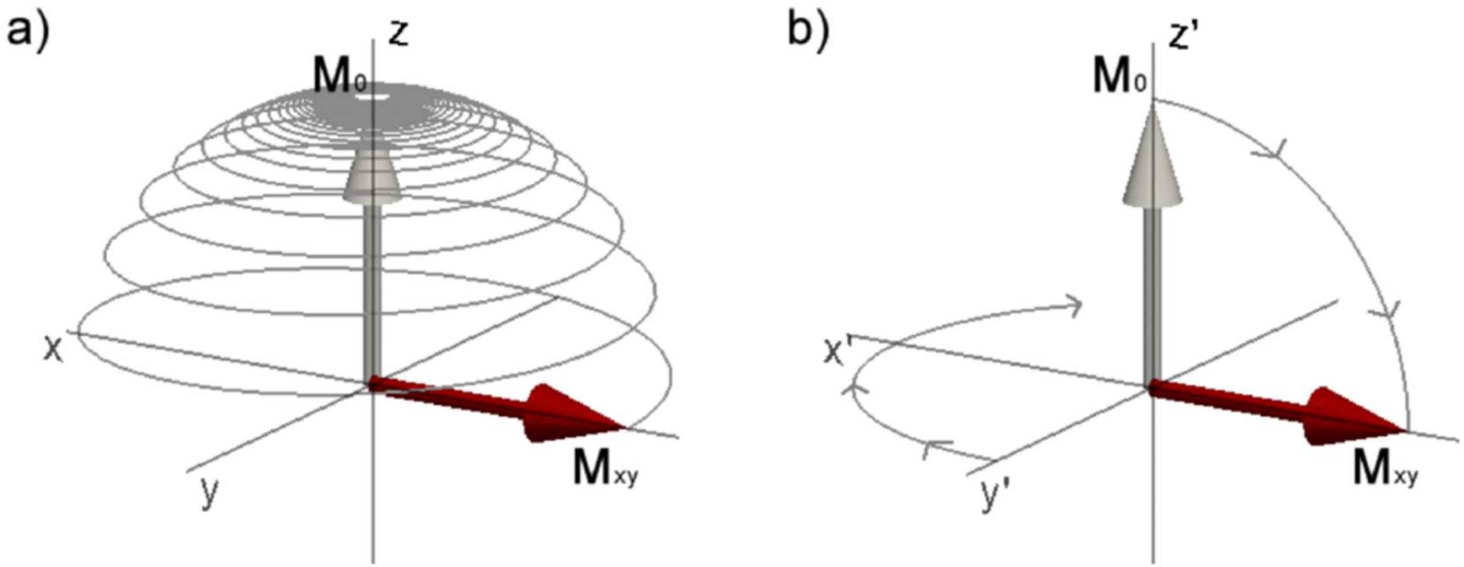
$$B_\perp = \left(B_\perp \sin \omega_L t\right) e_x + \left(B_\perp \cos \omega_L t\right) e_y \quad \Rightarrow \quad \theta(t) = \frac{2\mu B_\perp}{\hbar} t$$

Magnetic resonance

Solution in the resonance $\omega = \omega_L$

$$\theta(t) = \frac{2\mu B_\perp}{\hbar} t$$

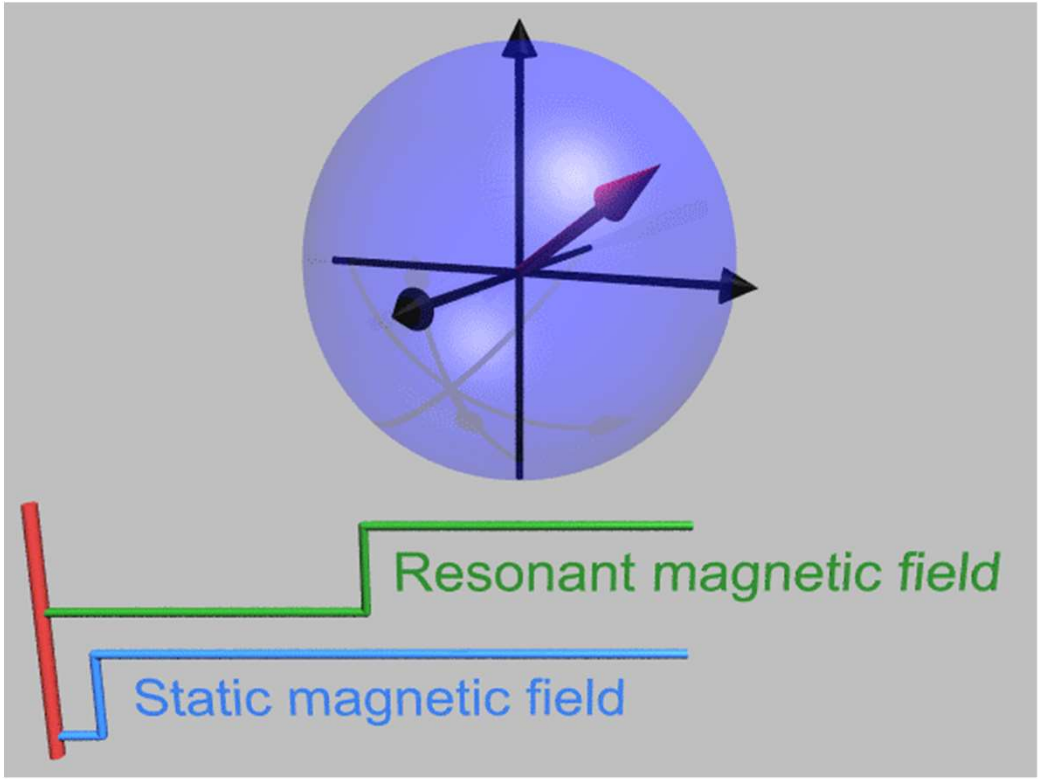
angle θ grows linearly in time



laboratory frame *rotating frame*

State of qubit changes from $|0\rangle$ to $|1\rangle$ and back periodically → ***Rabi oscillations***

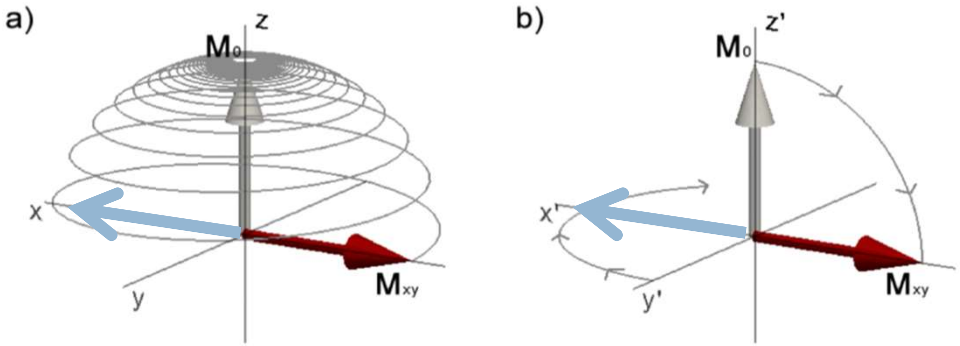
Magnetic resonance



Magnetic resonance

- ***Rabi oscillations***

$$\theta(T_R) = 2\pi = \frac{2\mu B_\perp}{\hbar} T_R \Rightarrow T_R = \frac{\pi\hbar}{\mu B_\perp} \Rightarrow \omega_R = \frac{2\pi}{T_R} = \frac{2\mu B_\perp}{\hbar} \ll \frac{2\mu B_\parallel}{\hbar} = \omega_L$$

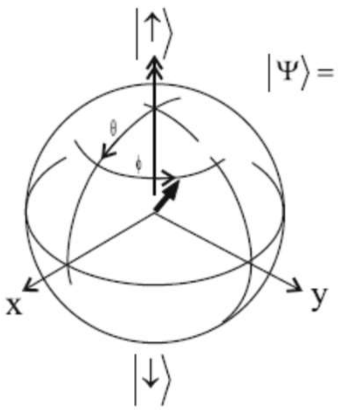


- On the return from $|1\rangle$ to $|0\rangle$ qubit is in the plane *xy* exactly in the opposite direction as was on the way from $|0\rangle$ to $|1\rangle$
- If we switch off $B_\perp$ at $\theta = \pi/2$ and wait half-period of ω_L, i.e. $\theta = 3\pi/2$, and switch on $B_\perp$ back → qubit will return directly to $|0\rangle$ without passing through $|1\rangle$

Quantum gates using pulses

a

Bloch-sphere representation



$$|\Psi\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + e^{i\phi}\sin\frac{\theta}{2}|\uparrow\rangle$$

$\theta = 0$ $\quad |\Psi\rangle = |\uparrow\rangle$

$\theta = \frac{\pi}{2}, \phi = 0$ $\quad |\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$

$\theta = \frac{\pi}{2}, \phi = \frac{\pi}{2}$ $\quad |\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$

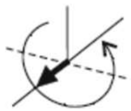
} superposition

$\theta = \pi, \phi = 0$ $\quad |\Psi\rangle = |\downarrow\rangle$

$\theta = 2\pi$ $\quad |\Psi\rangle = -|\uparrow\rangle$

property of spinor

$\theta = 4\pi$ $\quad |\Psi\rangle = |\uparrow\rangle$



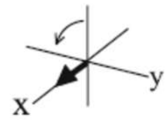
b

Manipulation of spin in the rotation frame by pulsed radiation field on resonance.

Generation of quantum gates by pulses

- $\pi/2$ x-pulse

$$|\uparrow\rangle \xrightarrow{P_x(\pi/2)} \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + i|\downarrow\rangle\right)$$



- $\pi/2$ y-pulse

$$|\uparrow\rangle \xrightarrow{P_y(\pi/2)} \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

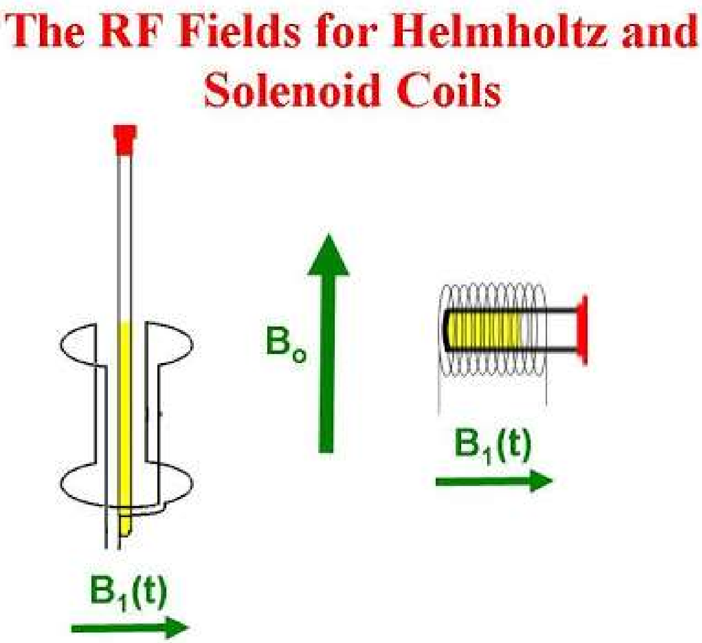
- π x-pulse

$$|\uparrow\rangle \xrightarrow{P_x(\pi)} -i|\downarrow\rangle$$

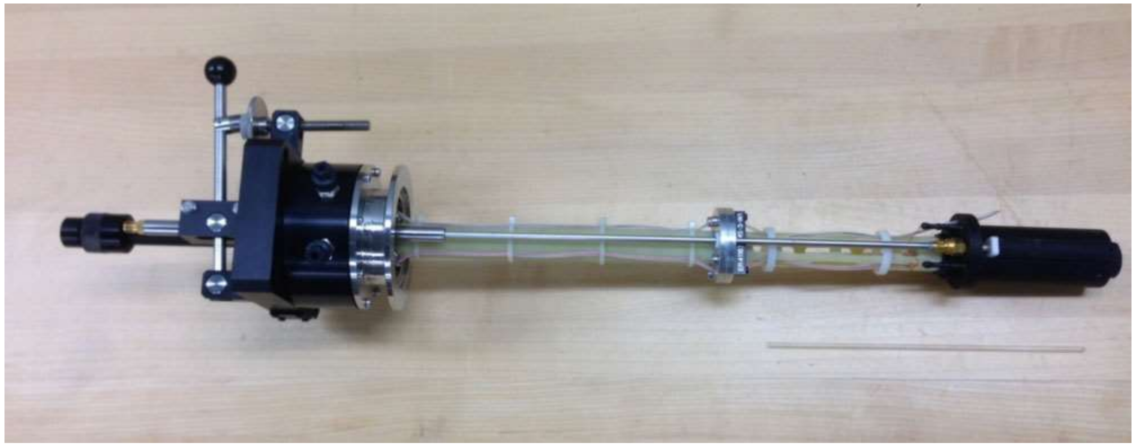
Detection of the state in MagRes

The state of vector – qubit – detected also in the direction perpendicular to *z*-axis, e.g. as induced voltage in the detection coil, which could be the same one as used for excitation

NMR



EPR



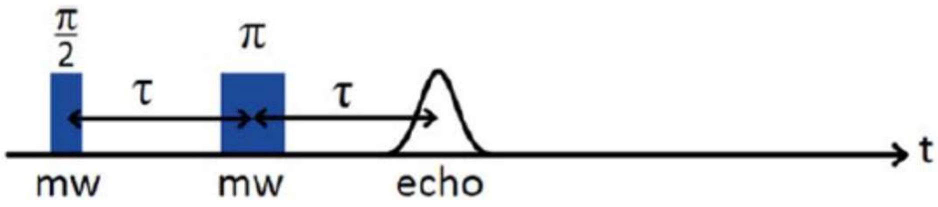
detection of electron paramagnetic resonance (EPR) in resonator

Decoherence again

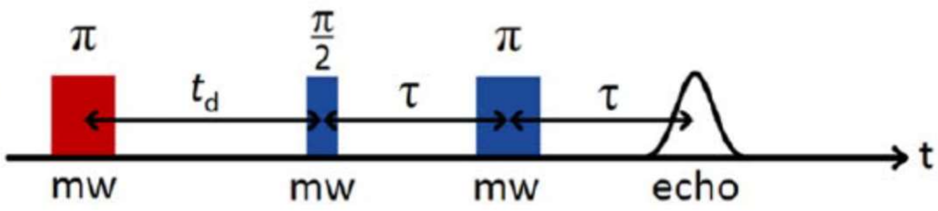
How to determine characteristic parameters describing the loss of quantum information using magnetic resonance ?

Measure T_1, T_2 a T_R

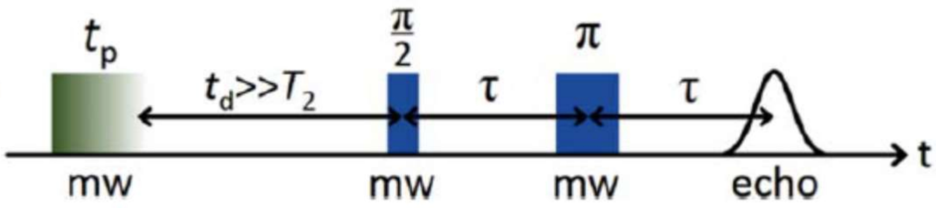
T_2 → Hahn-echo



T_1 → Inversion recovery



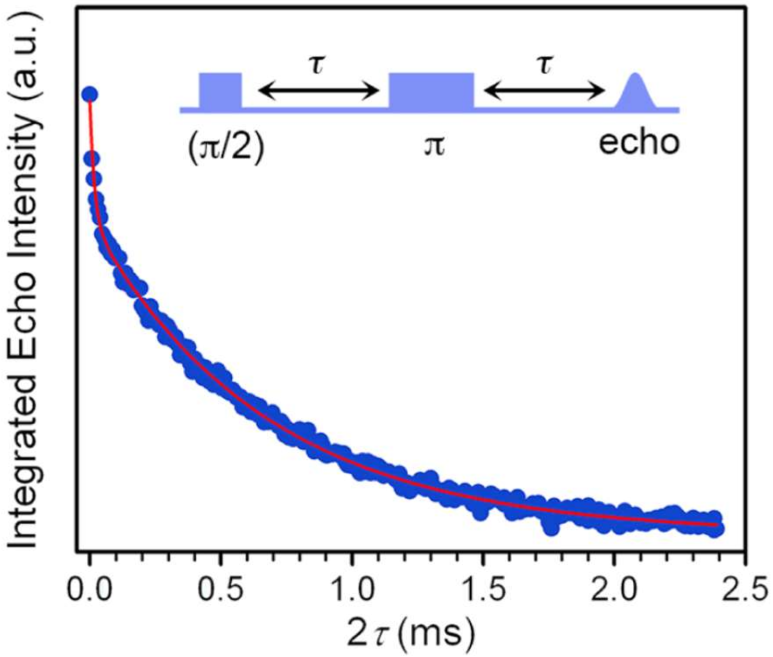
T_R → Transient nutation



Hahn echo

Determination of quantum coherence time

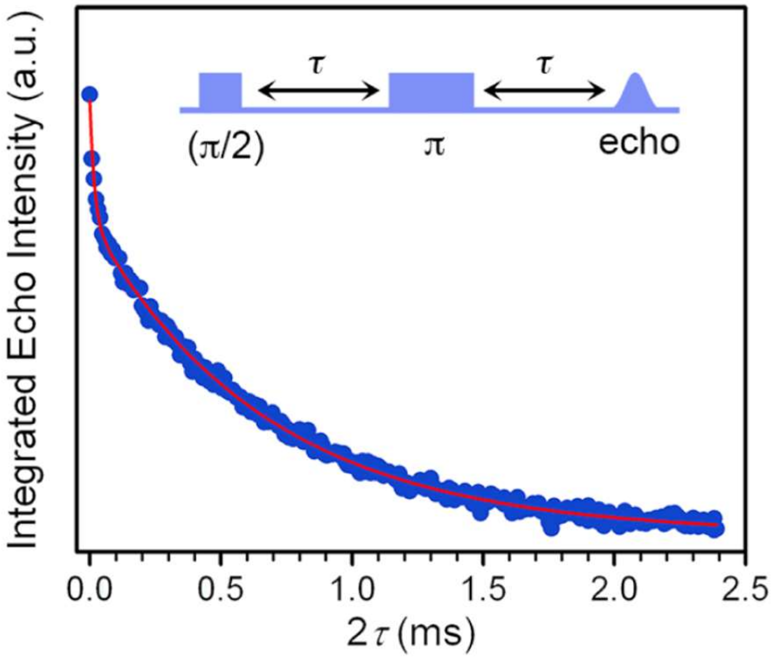
Pulsed EPR – sequence of microwave pulses (or radio-frequency for NMR) – dependence of spin echo intensity on the delay between pulses depends exponentially on $\boldsymbol{T_2}$

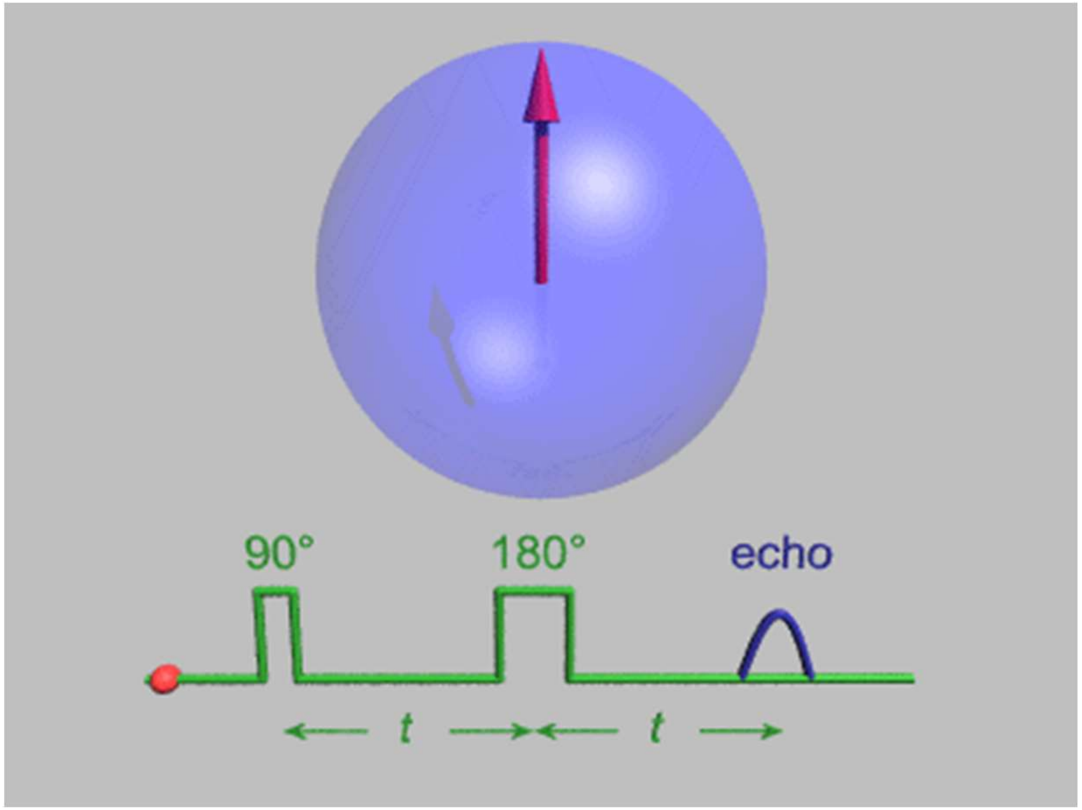


Hahn echo

Determination of quantum coherence time

*Pulsed EPR – sequence of microwave pulses (or radio-frequency for NMR) – dependence of spin echo intensity on the delay between pulses depends exponentially on **T_2***

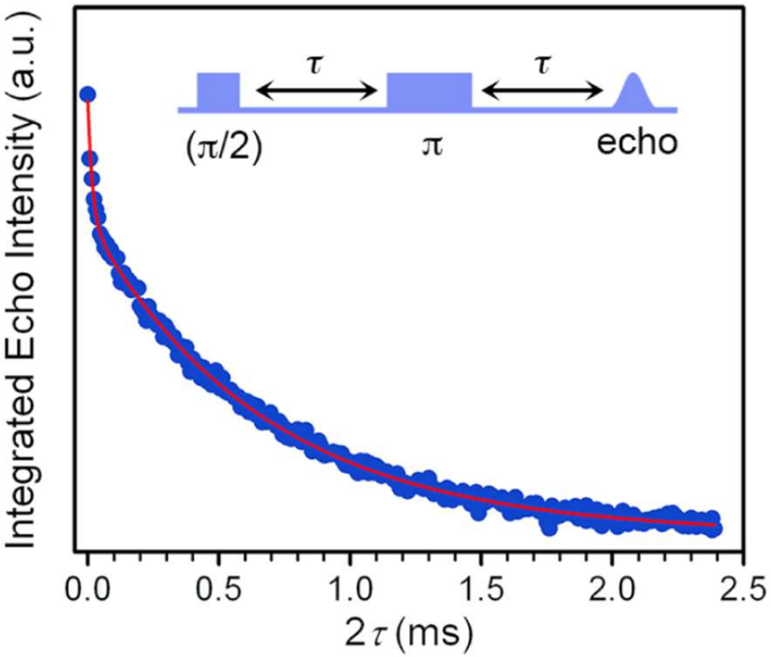


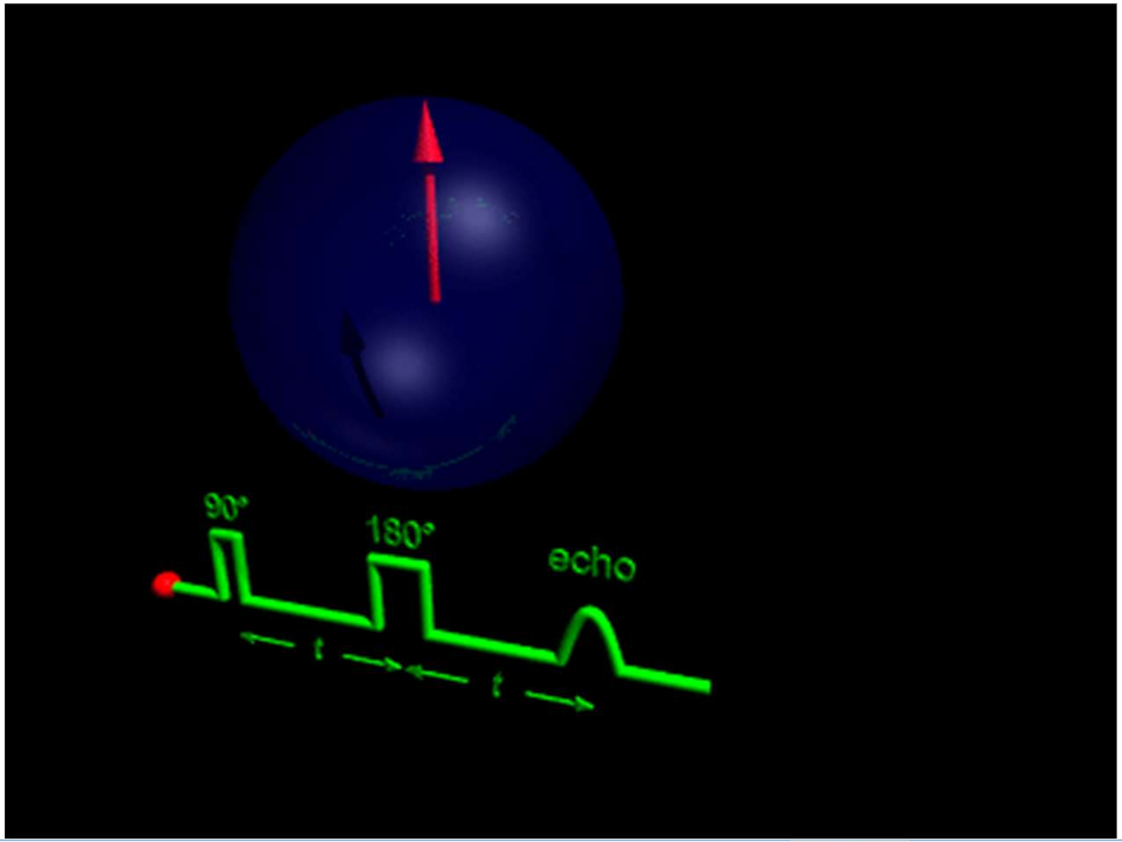


Hahn echo

Determination of quantum coherence time

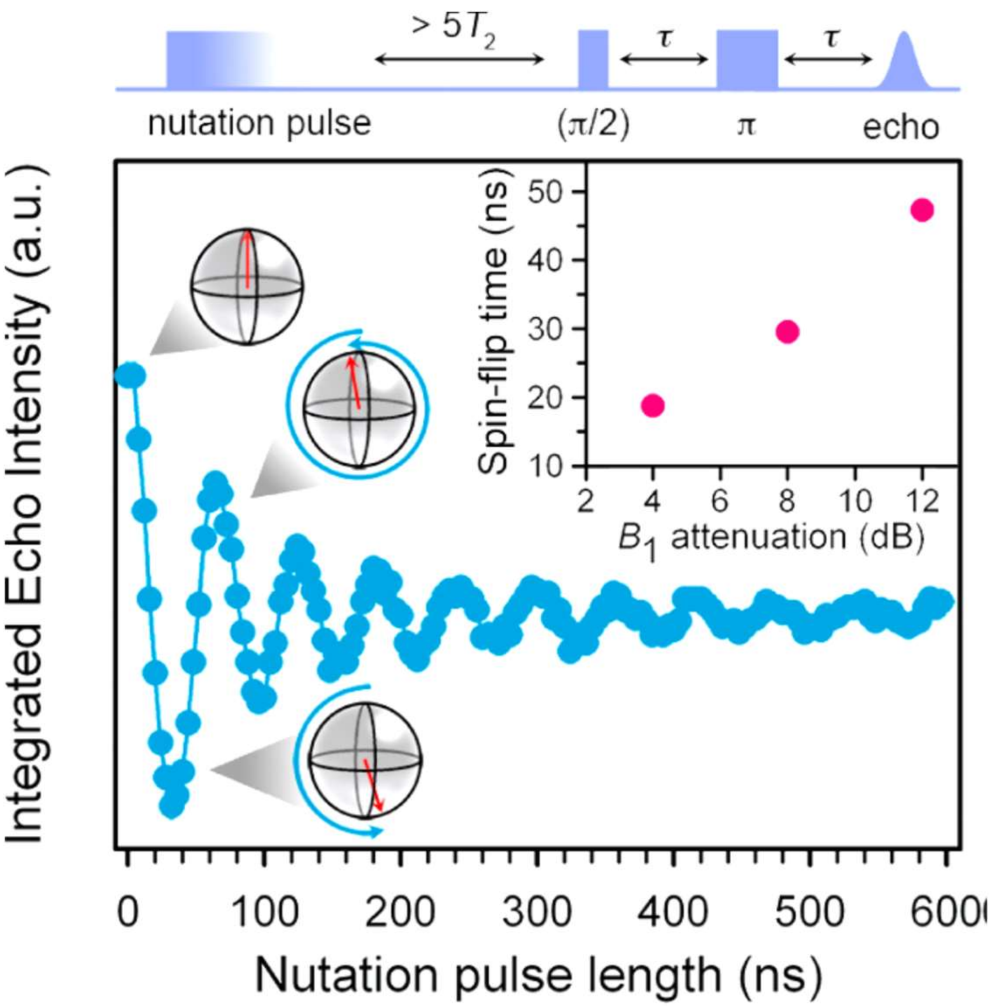
Pulsed EPR – sequence of microwave pulses (or radio-frequency for NMR) – dependence of spin echo intensity on the delay between pulses depends exponentially on $\boldsymbol{T_2}$





Rabi oscillations

- *Period of oscillations defines spin-flip time – NOT gate*
- *Ratio of T_2/T_R (qubit figure of merit) represents the number of operations we can perform during T_2*

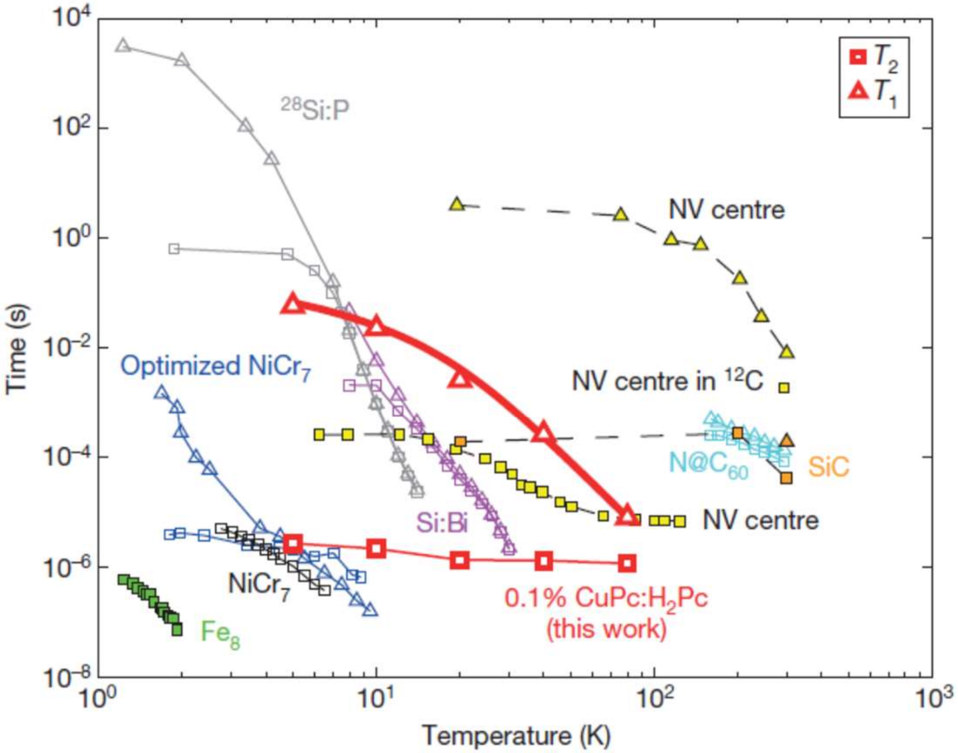


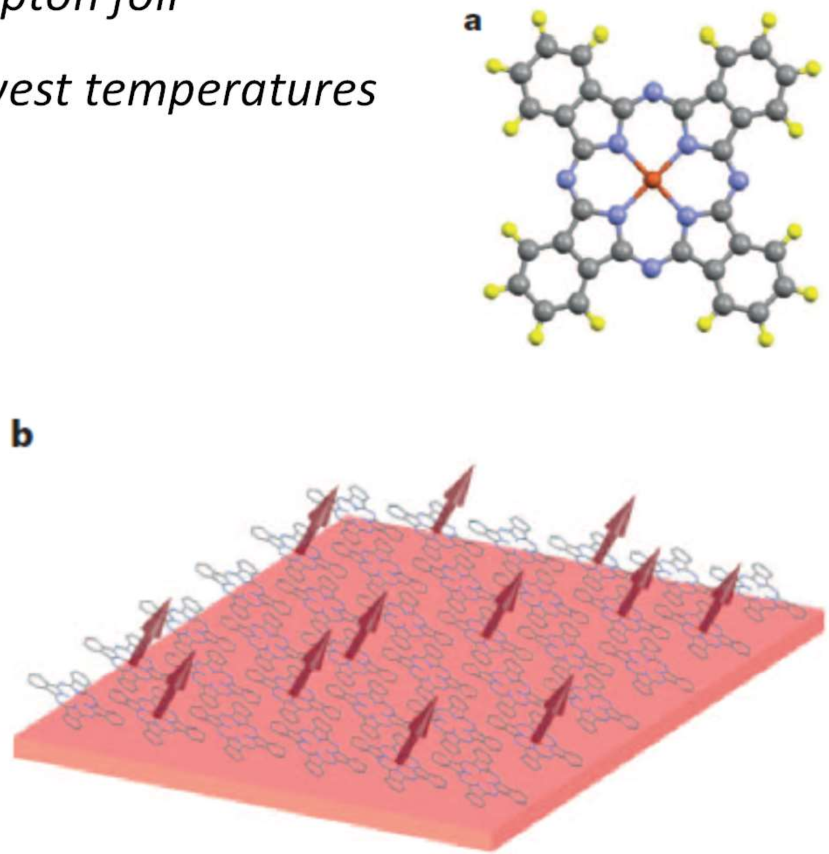
Single-ion magnets

- *Thin layer diluted Cu-phthalocyanine on Kapton foil*

T_2 = 1 μs @ 77 K, almost constant down to lowest temperatures

Nature 503 (2013) 504





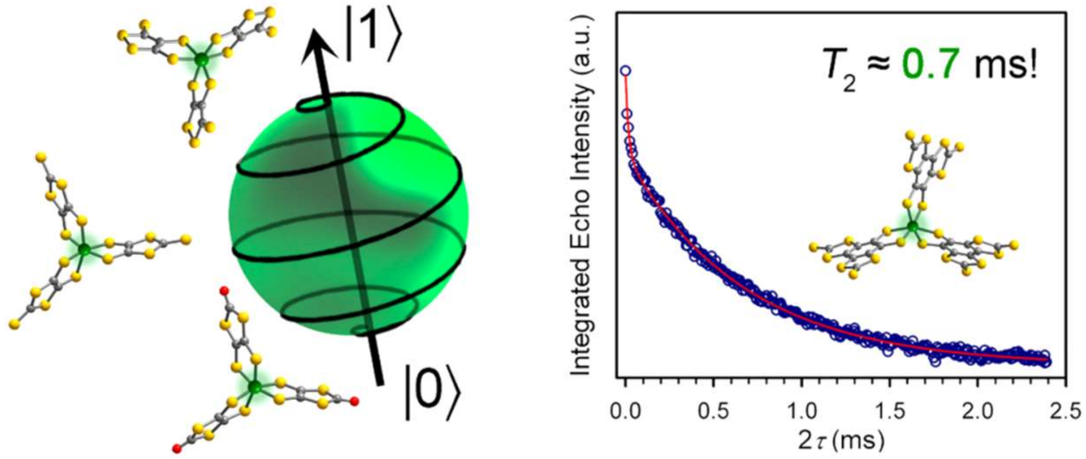
Single-ion magnets

- *$(d_{20}\text{-}Ph_4P)_2[V(C_8S_8)_3]$ in solution of CS_2*

  T_2 = 0.7 ms @ 10 K

  T_2 = 1 μ s @ 300 K

ACS Cent. Sci. 1 (2015) 488



- Presence of nuclear spin accelerates decoherence – spin-flops of nuclear spins create time-dependent fields at the electron site yielding to decoherence

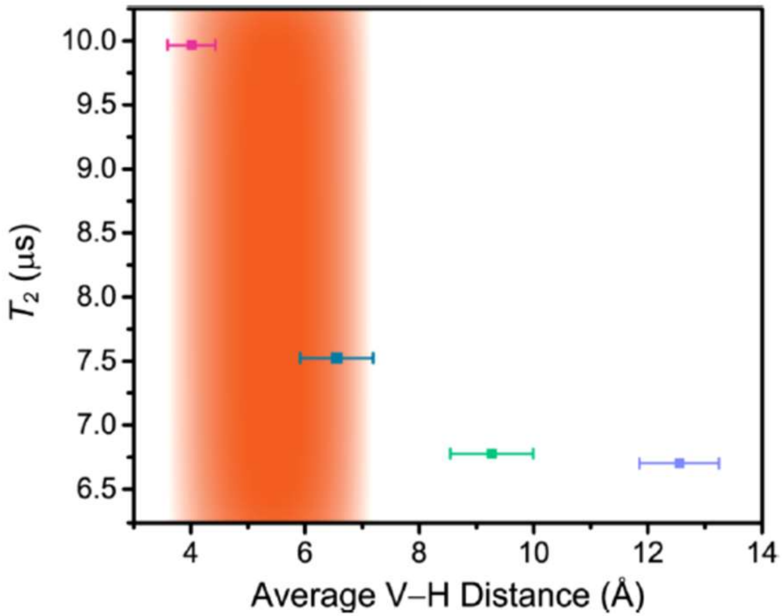
Single-ion magnets

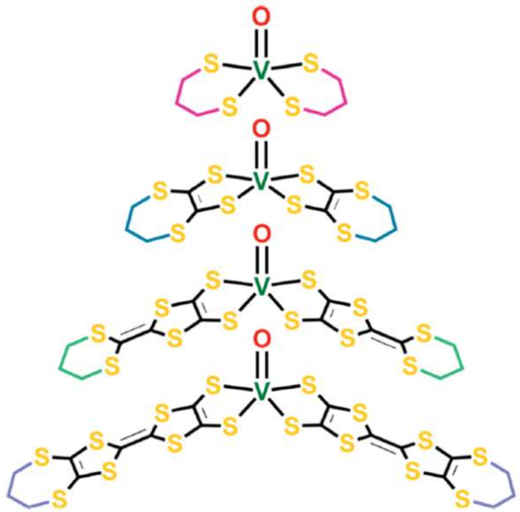
- Does the presence of nuclear spin indeed accelerate decoherence?

Synthetic Approach To Determine the Effect of Nuclear Spin Distance on Electronic Spin Decoherence

Michael J. Graham,† Chung-Jui Yu,† Matthew D. K
and Danna E. Freedman*,†

DOI: 10.1021/jacs.6b13030
J. Am. Chem. Soc. 2017, 139, 3196–3201



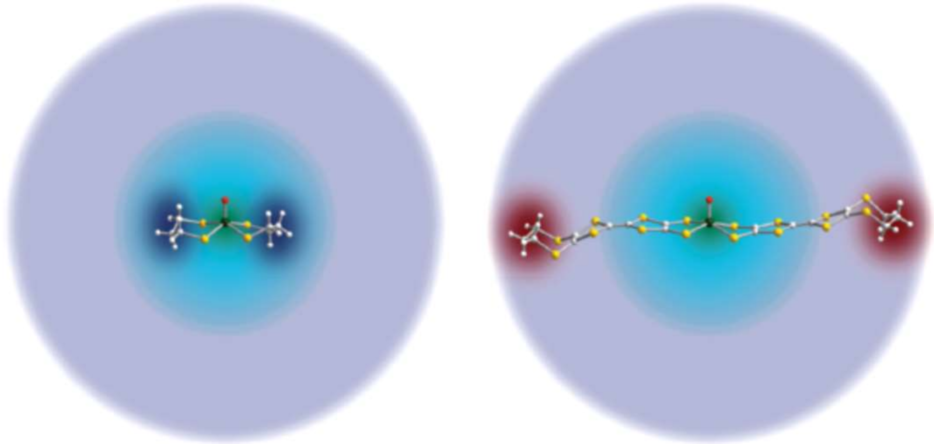


Single-ion magnets

- Does the presence of nuclear spin indeed accelerate decoherence?

DOI: 10.1021/jacs.6b13030
J. Am. Chem. Soc. 2017, 139, 3196–3201

- ***T_1 remains the same, but T_2 not*** – **nuclear spin diffusion barrier radius** – nuclei inside this barrier are too strong coupled to electrons to perform spin-flops and do not contribute to decoherence (prediction from 1947)



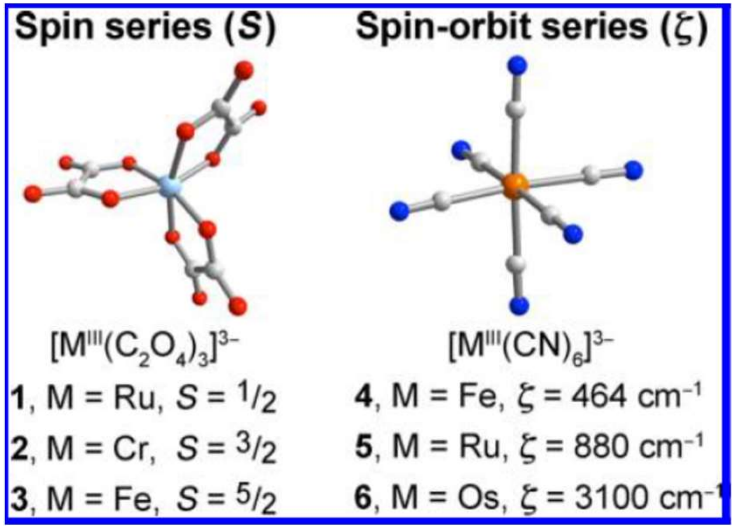
Single-ion magnets

- Does decoherence depend on spin value and spin-orbit coupling?

Influence of Electronic Spin and Spin–Orbit Coupling on Decoherence in Mononuclear Transition Metal Complexes

Michael J. Graham,[†] Joseph M. Zadrozny,[†] Muhandis Shiddiq,[‡] John S. Anderson,[†] Majed S. Fataftah,[†] Stephen Hill,*[,‡] and Danna E. Freedman*[,†]

dx.doi.org/10.1021/ja5037397 | J. Am. Chem. Soc. 2014, 136, 7623–7626



	1	2	3
S	$^1/_2$	$^3/_2$	$^5/_2$
H_{dc} (Oe)^b	2812	2130	3501
T_2 at 5 K	3.44(1)	2.79(3)	1.83(1)
T_2 at 14 K	2.01(1)	1.86(3)	0.81(1)
T_2 at 22 K	0.41(2)	1.27(4)	0.45(5)
	4	**5**	**6**
S	$^1/_2$	$^1/_2$	$^1/_2$
ζ (cm^{-1})^c	464	880	3100
H_{dc} (Oe)^b	3364	3394	3865
T_2 at 5 K	2.38(6)	2.55(4)	4.12(6)
T_2 at 13 K	0.55(8)	1.25(5)	3.17(4)
T_2 at 22 K	0.60(9)	1.29(10)	1.04(4)

Single-ion magnets

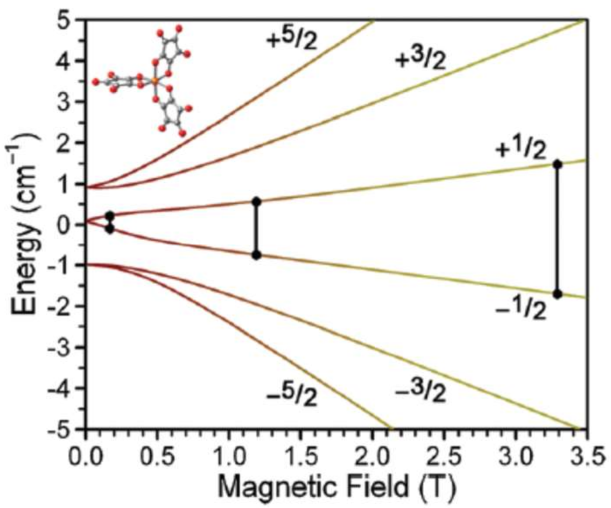
- Long coherence time with high-spin ion?

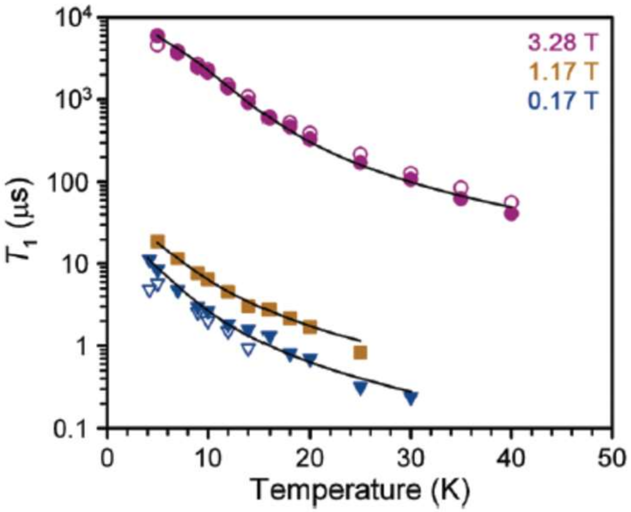
Unexpected suppression of spin–lattice relaxation *via* high magnetic field in a high-spin iron(III) complex†

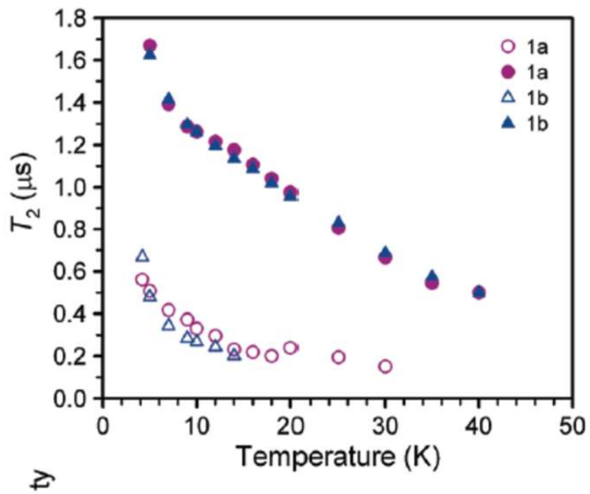
Joseph M. Zadrozny,[a] Michael J. Graham,[a] Matthew D. Krzyaniak,[ab] Michael R. Wasielewski[ab] and Danna E. Freedman*[a]

ChemComm
Cite this: DOI: 10.1039/c6cc05094h
Received 17th June 2016,
Accepted 21st July 2016

- High-spin Fe(III) complex in strong magnetic field – suppression of the spin state mixing







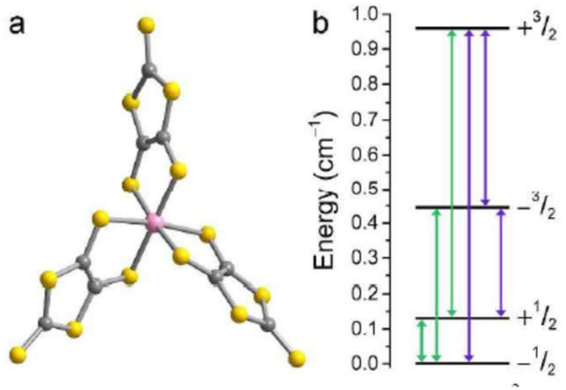
Single-ion magnets

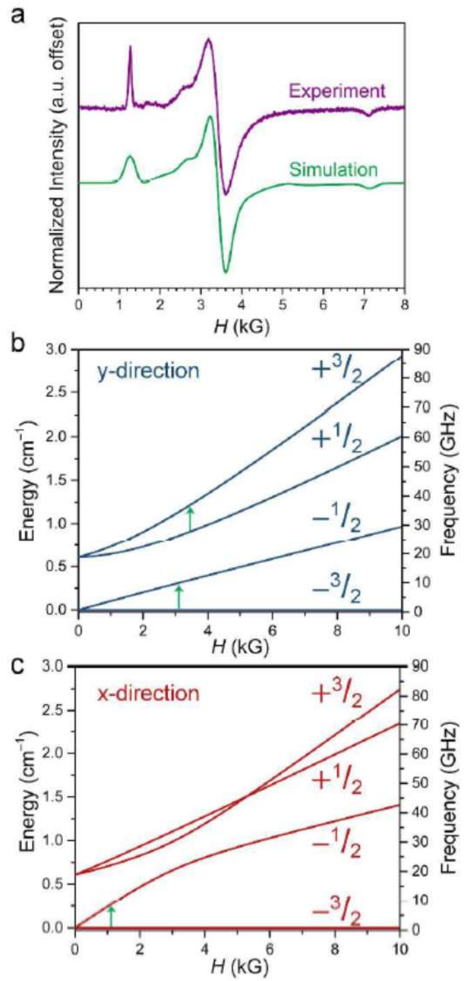
- Use more spin transitions within one set of energy levels?

Employing Forbidden Transitions as Qubits in a Nuclear Spin-Free Chromium Complex

Majed S. Fataftah, Joseph M. Zadrozny, Scott C. Coste, Michael J. Graham, Dylan M. Rogers, and Danna E. Freedman

J. Am. Chem. Soc., **Just Accepted Manuscript** • DOI: 10.1021/jacs.5b11802 • Publication Date (Web): 07 Jan 2016





Single-ion magnets

- Use more spin transitions within one set of energy levels?

Employing Forbidden Transitions as Qubits in a Nuclear Spin-Free Chromium Complex

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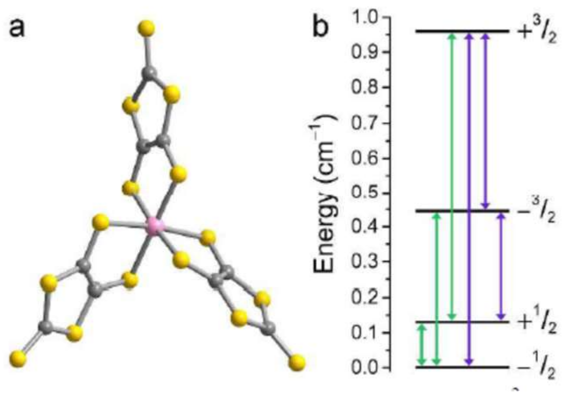
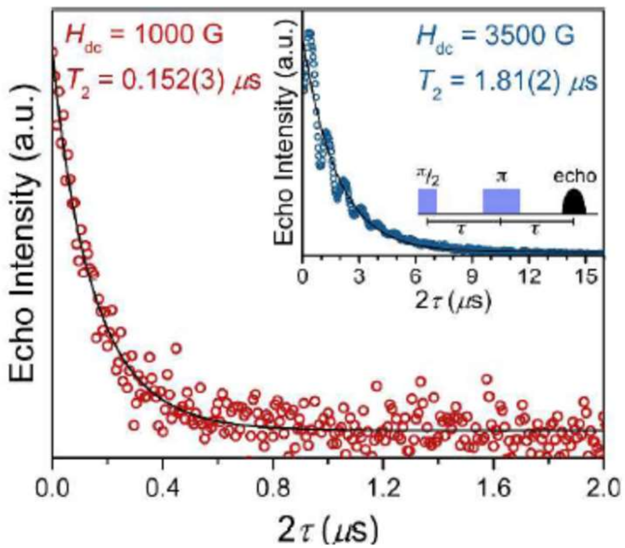
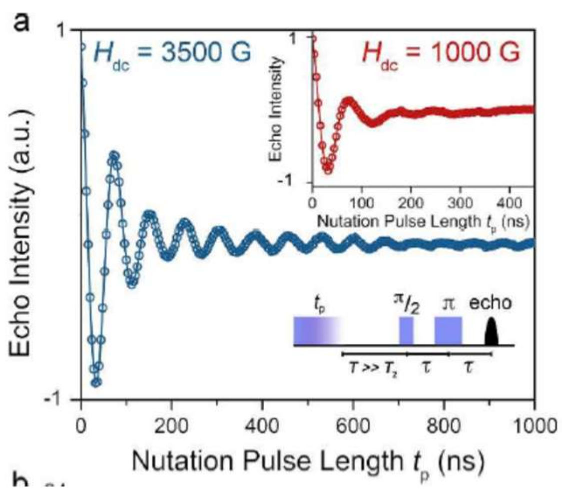
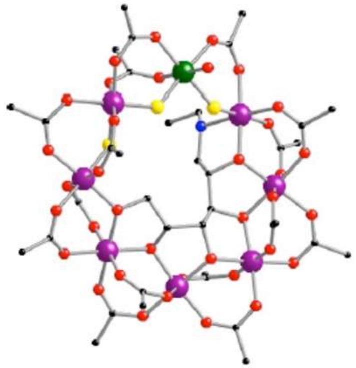


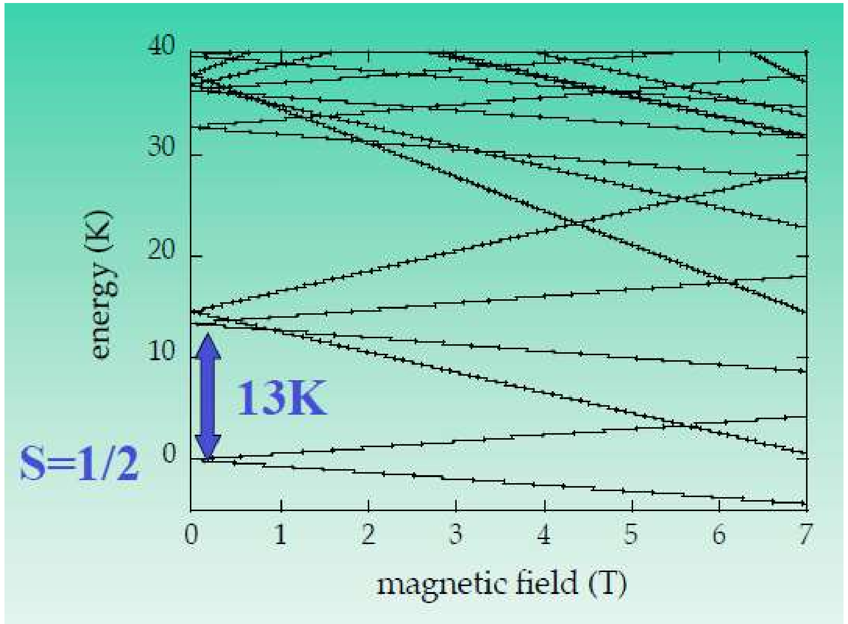




Molecular spin clusters

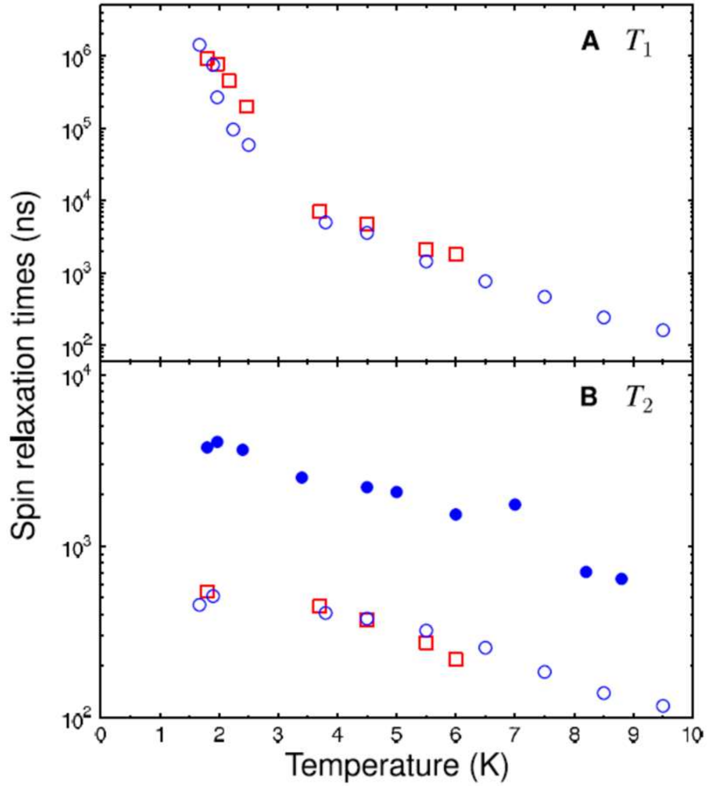
Cr_7Ni ring (Affronte, Winpenny et al.)





T_2 = 3 μs, deuterated sample

PRL 98 (2007) 057201

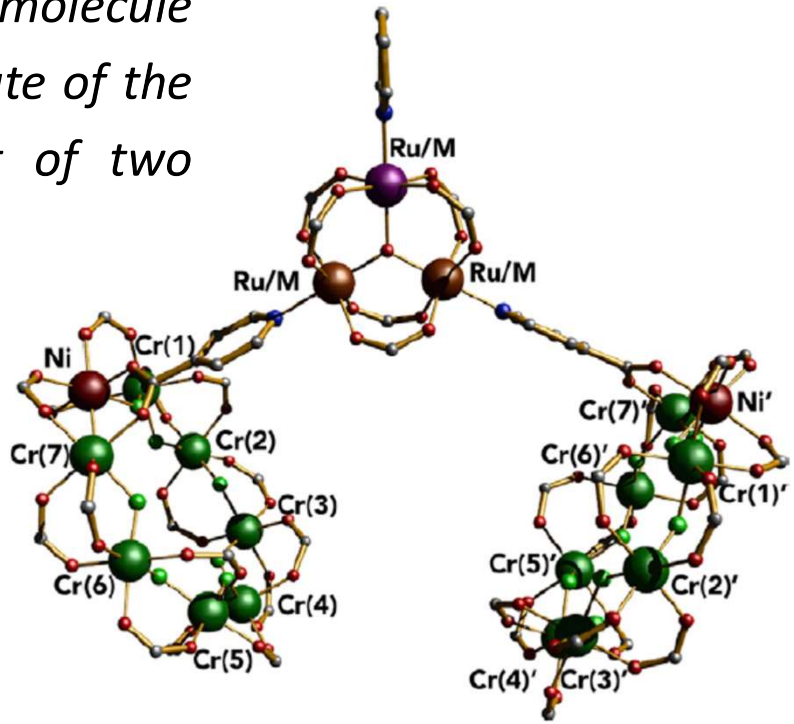


Molecular spin clusters

Quantum entanglement in Cr_7Ni – Ru_2Co^{2+} - Cr_7Ni (Affronte, Winpenny et al.)

Nat. Nanotech. (2009) 173

- *By injecting or removing electron from molecule (e.g. from STM tip) we change the spin state of the link – separation or back entanglement of two qubits based on Cr_7Ni rings*
- *Realization of $\sqrt{iSWAP}$ gate*



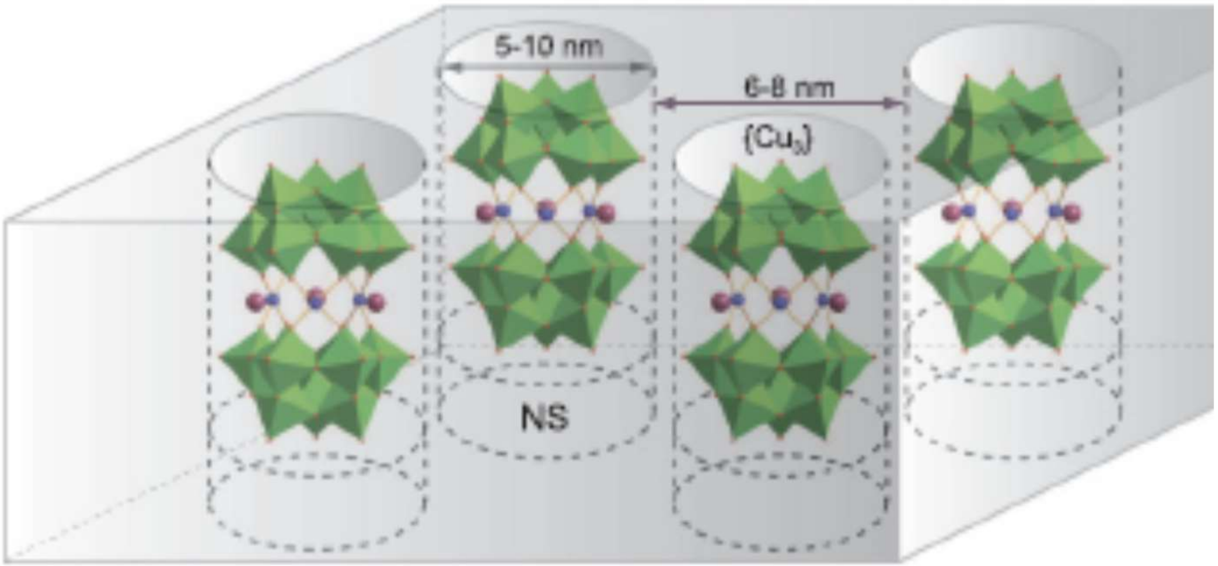
Molecular spin clusters

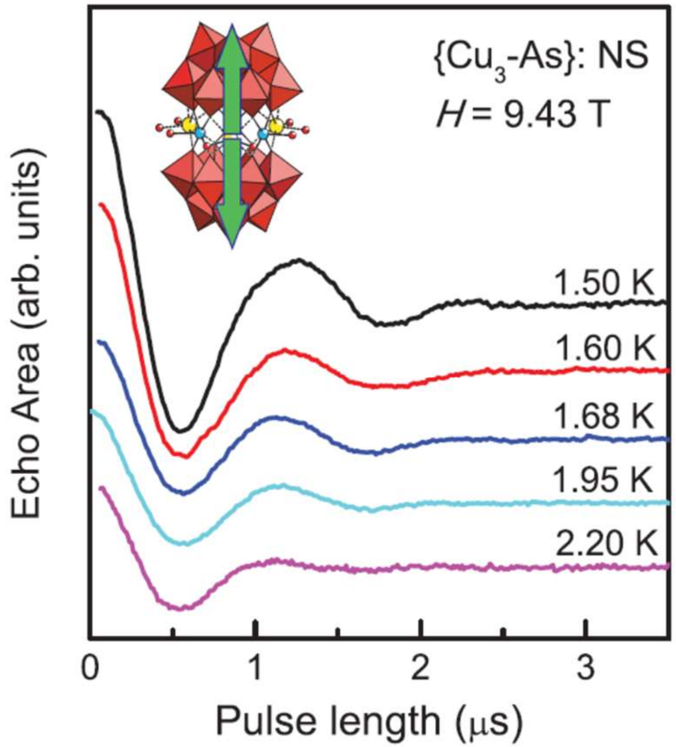
- *Spin trimer based on S=1/2 Cu^{2+} ions*

$Na_{12}[X_2W_{18}Cu_3O_{66}(H_2O)_3].32H_2O$ (X - As, Sb) in nanoporous silica

$T_2 = 3\ \mu s$

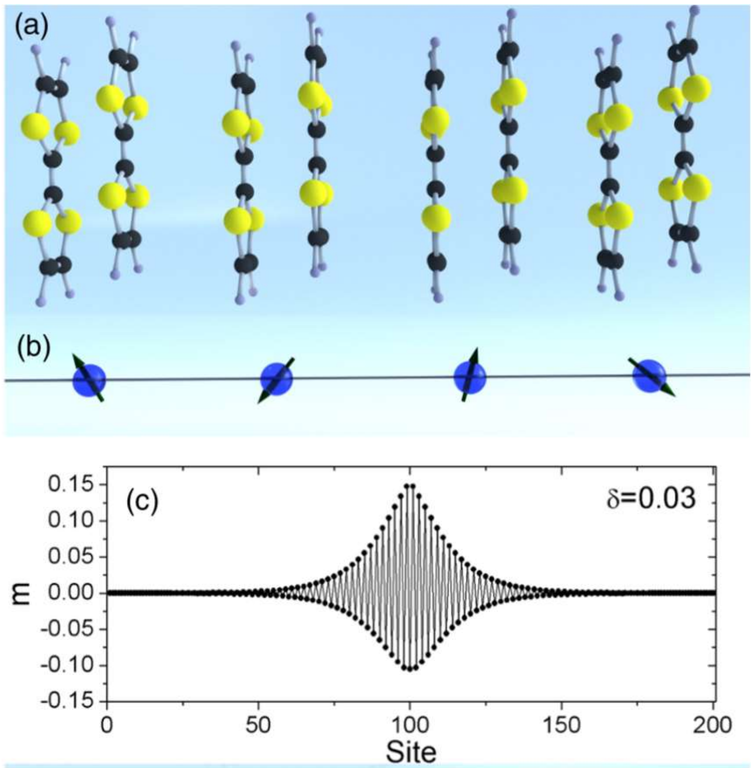
PRL 108 (2012) 067206

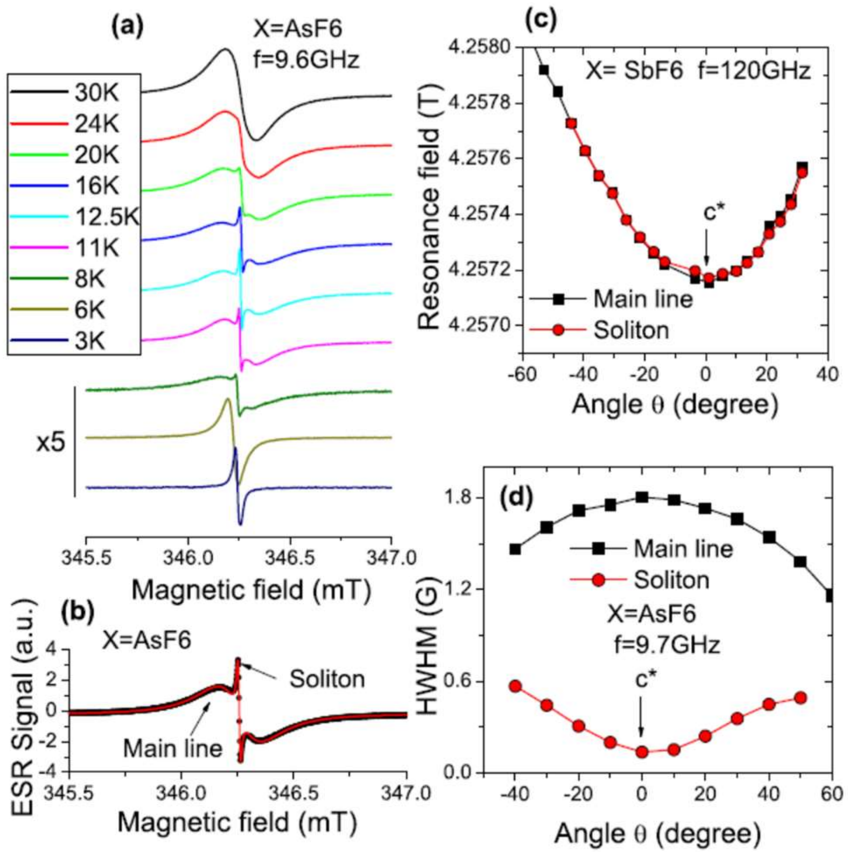




Quantum bits in spin chains

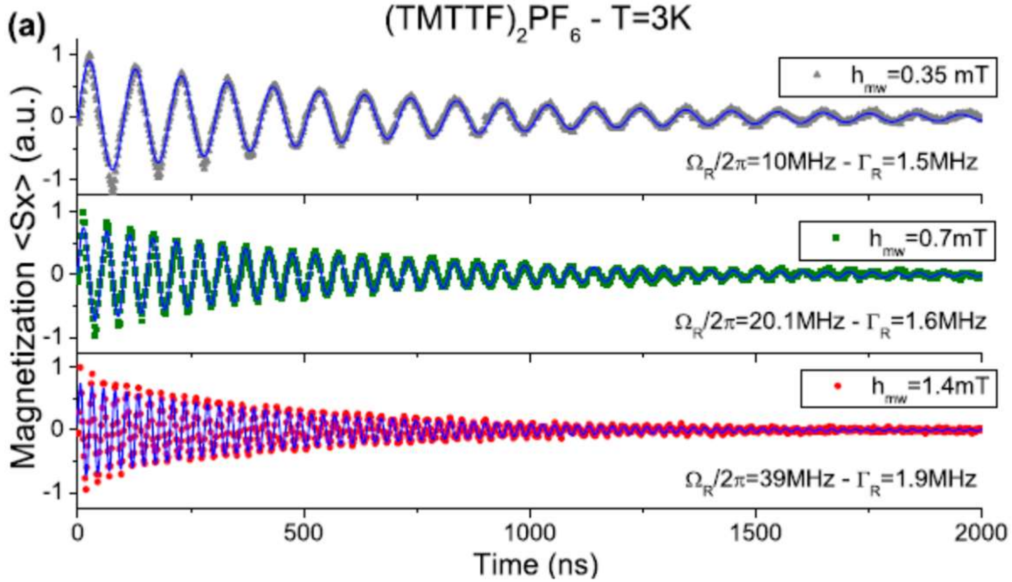
- ***dimerized AFM spin chain - $(TMTTF)_2X$, where X = AsF_6, PF_6, SbF_6***
- *defect generates a local change of exchange interaction, localized magnetic object with spin ½ created - soliton PRB 90 (2014) 060404(R)*





Quantum bits in spin chains

- *Rabi oscillation*



Solitons are trapped at defect site in chain

- *Strong isotropic exchange interaction (about 400 K) between qubits generates narrow and homogenous EPR lines (exchange narrowing, well defined)*
- *Suppressed sources of decoherence related to inhomogeneity of local field (to avoid non identical qubits) or dipole-dipole interactions*
- *It is possible to work with high energy microwave pulses (usually coherence quickly decays in other magnets for high power pulses)*
- *Possibility of quantum entanglement through strong exchange interaction along the chain*

Something new?

SCIENCE ADVANCES | RESEARCH ARTICLE

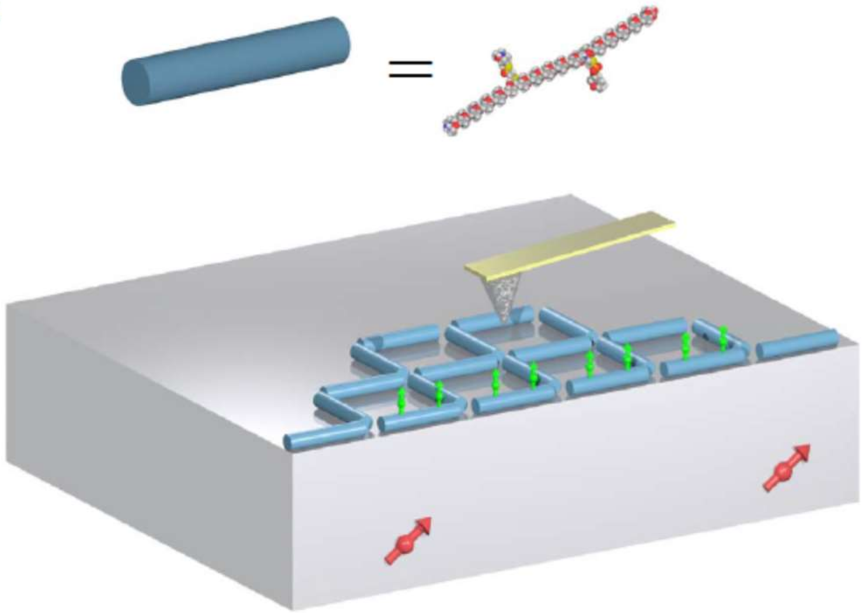
QUANTUM INFORMATION

Sci. Adv. 2017;**3**:e1701116

A molecular quantum spin network controlled by a single qubit

Lukas Schlipf,[1,2] Thomas Oeckinghaus,[2] Kebiao Xu,[1,2,3] Durga Bhaktavatsala Rao Dasari,[1,2] Andrea Zappe,[2] Felipe Fávaro de Oliveira,[2] Bastian Kern,[1] Mykhailo Azarkh,[4] Malte Drescher,[4] Markus Ternes,[1] Klaus Kern,[1,5] Jörg Wrachtrup,[1,2] Amit Finkler[2]*

A

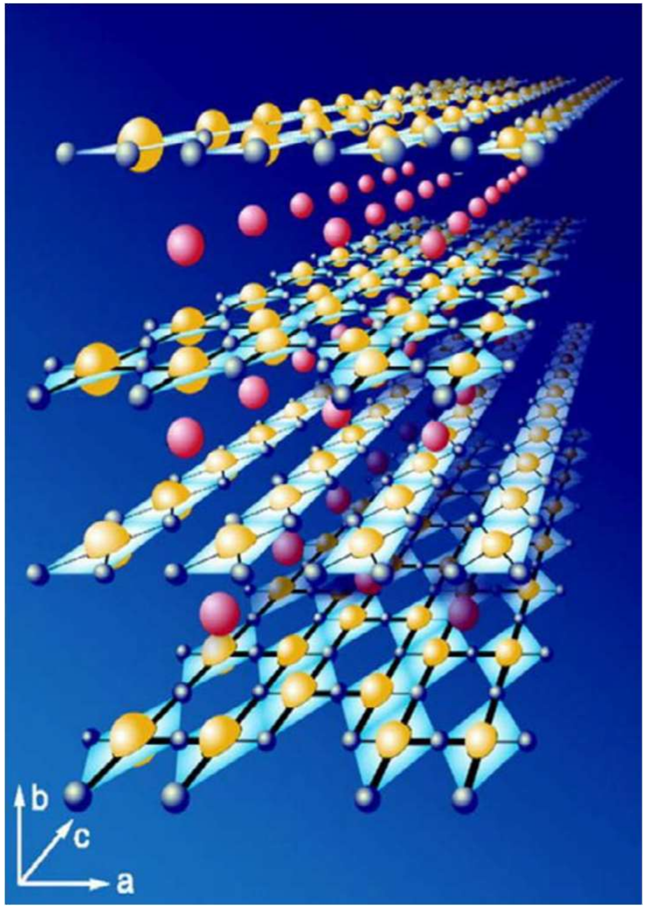


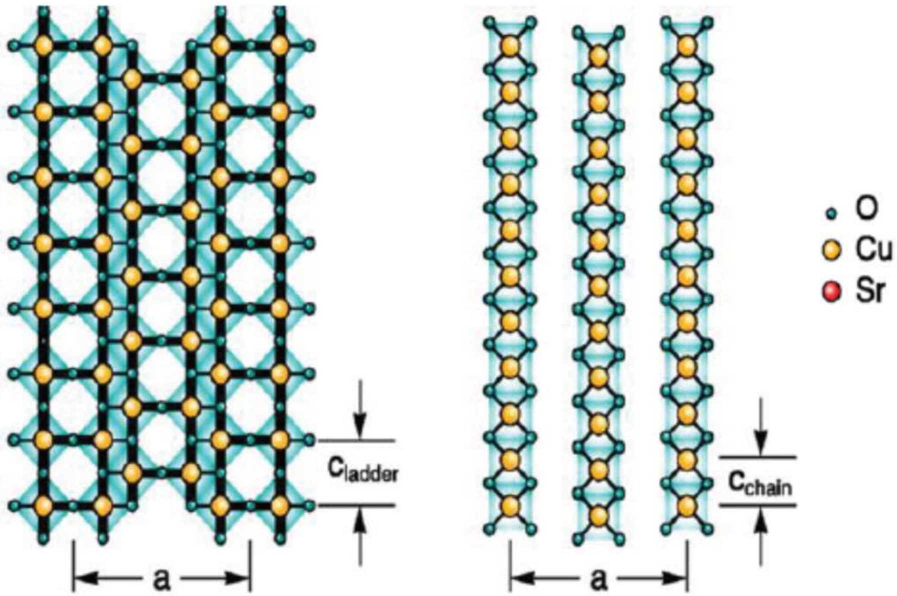
- „Spin-labeled" peptides on 30μm diamond with implanted NV-centres (defects)
- MW pulse manipulates spin in peptide
- NV center detects the quantum state of the spin in peptide and this is detected from fluorescence of NV-center using confocal microscope
- It is possible to detect signal from one NV-center

Entanglement in spin chains

$Sr_{14}Cu_{24}O_{41}$

Nat. Phys. 11 (2015) 255

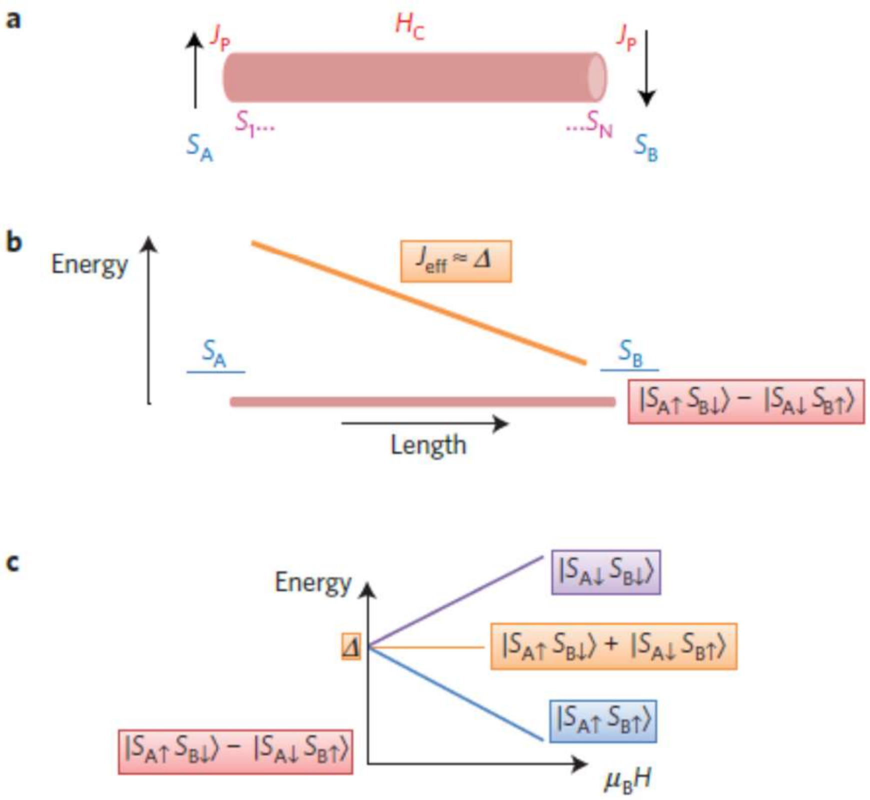


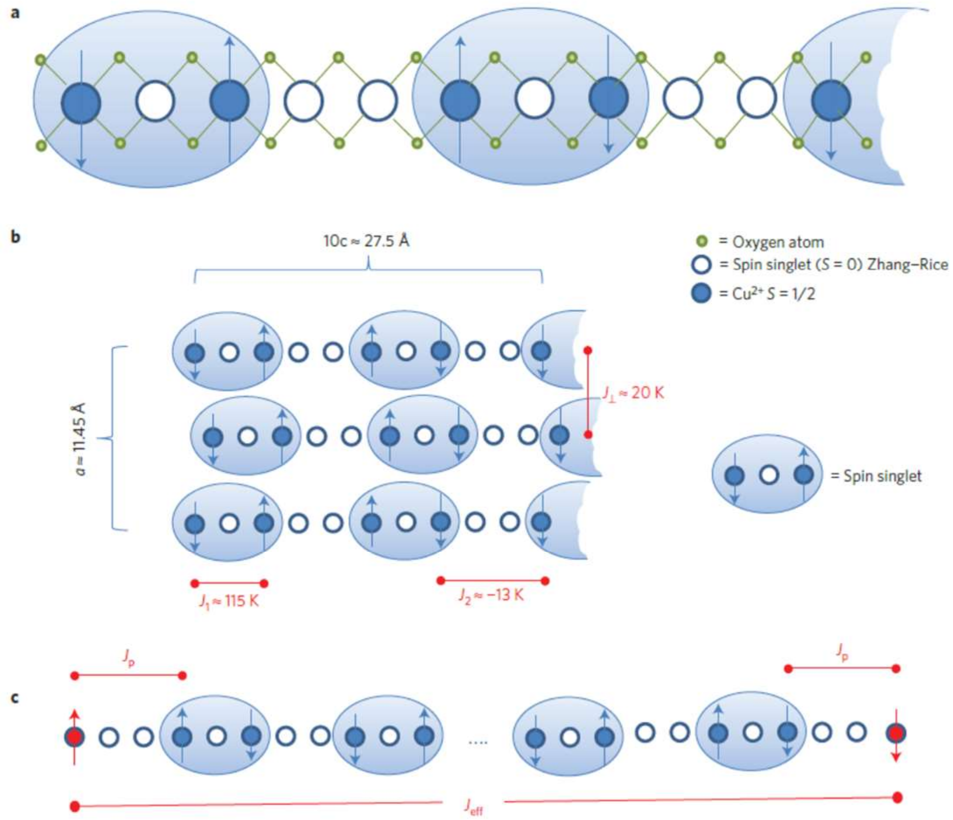


$7c_{ladders} \approx 10c_{chains}$

Entanglement in spin chains

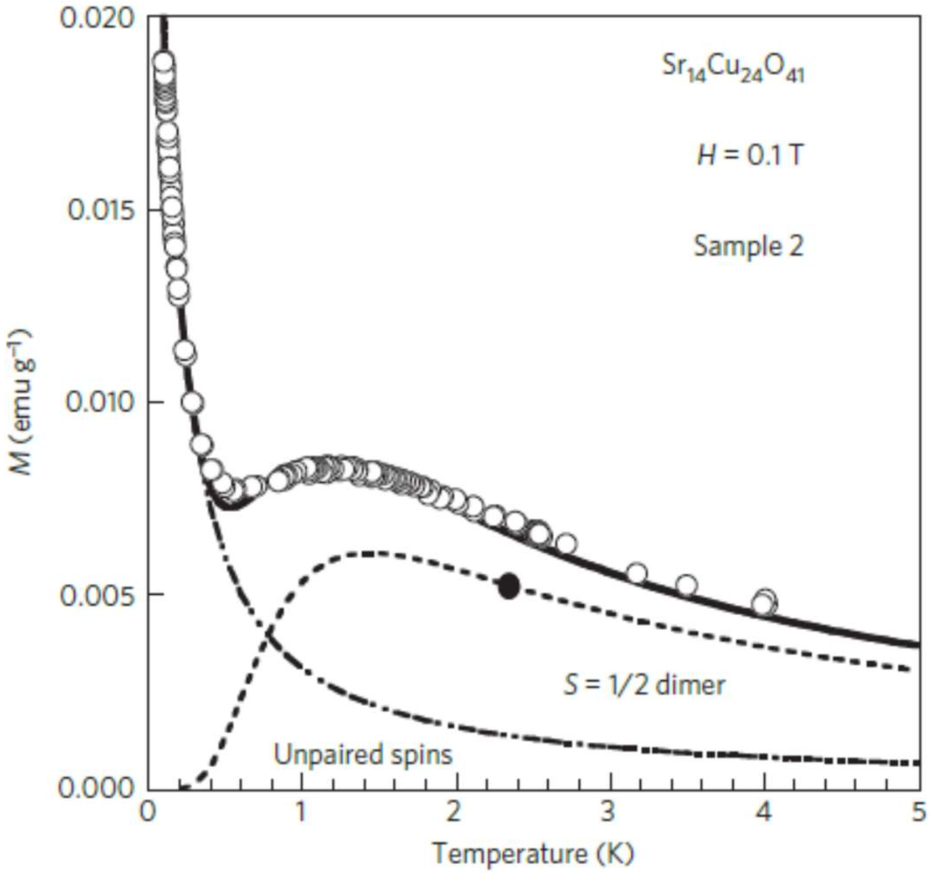
- *Incommensurability between ladder and chain layer creates S=1/2 states in dimerized chain*





Entanglement in spin chains

- *Long-distance entanglement between induced S=1/2 objects at low temp.*



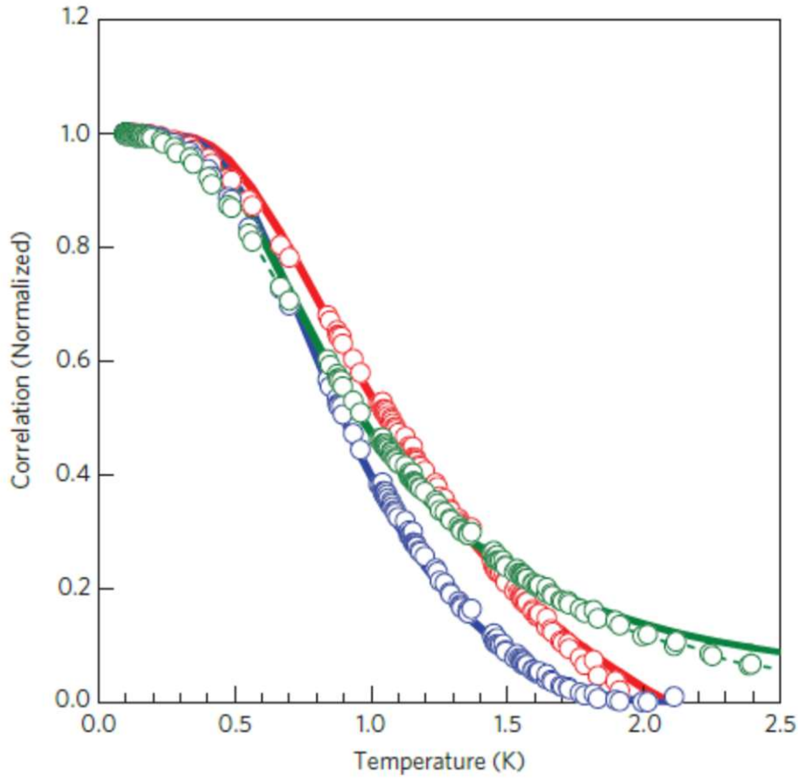


Figure 5 | Quantum correlations. Concurrence (red), entanglement (blue) and quantum information (green) correlations as a function of temperature. Data (in circles) are extracted from Fig. 3a, once the Curie tail has been subtracted. The calculations (solid lines) correspond to the spin-dimer model[21,42].

The End