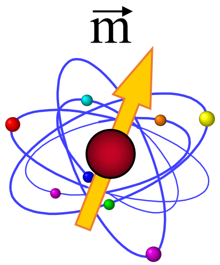
Lecture 9

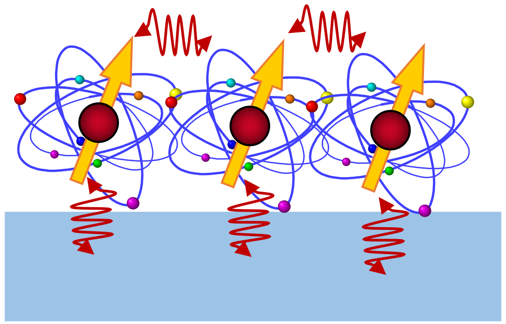
Spin dynamics and spin-transfer-torque at atomic scale

The spintronics “goose game”

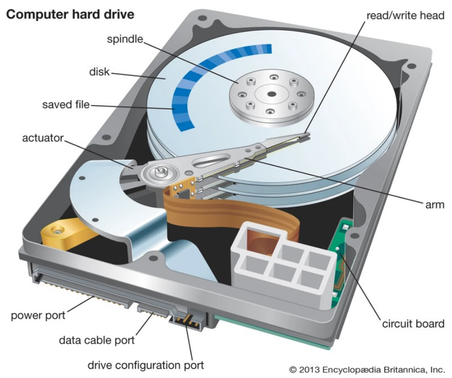
Atom magnetism

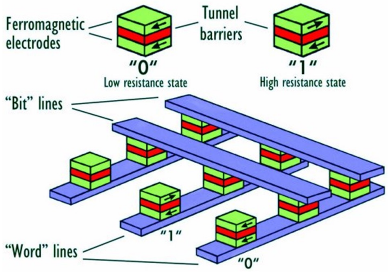


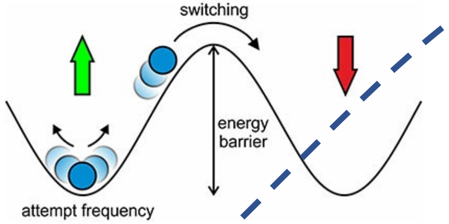
interactions between spins and with the supporting substrate



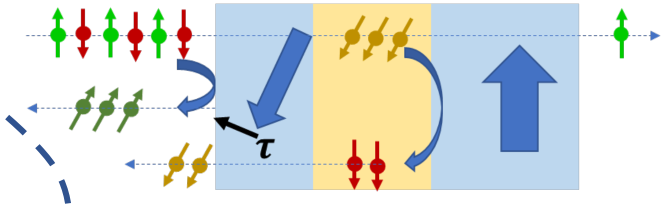
applications

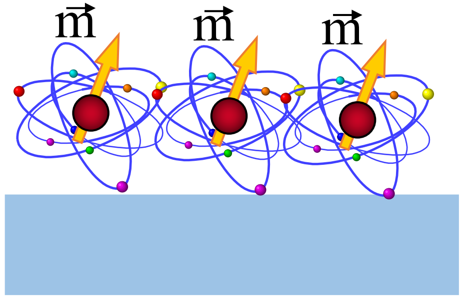




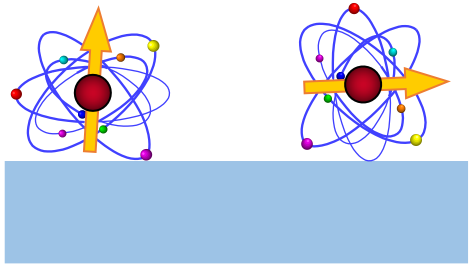


STT - SOT



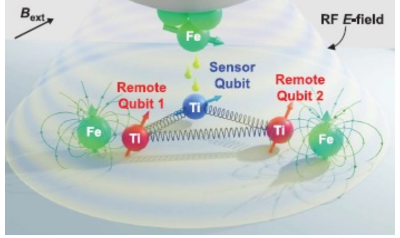


magnetic moment in a cluster and/or on a support

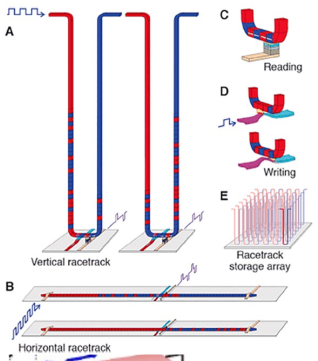


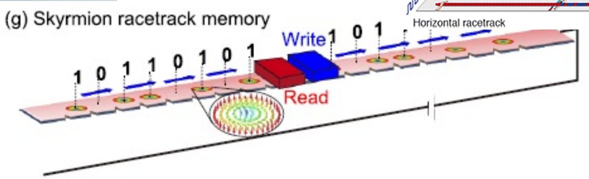
Magnetization easy axis

Quantum objects

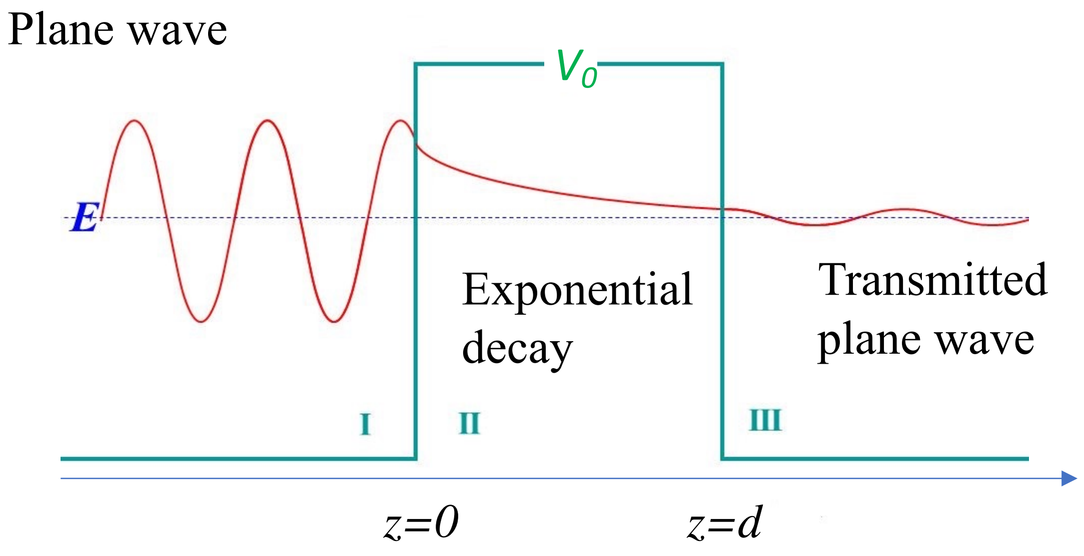


Future





Scanning tunneling microscopy (STM)



in region II (classically forbiden), exponential decay:

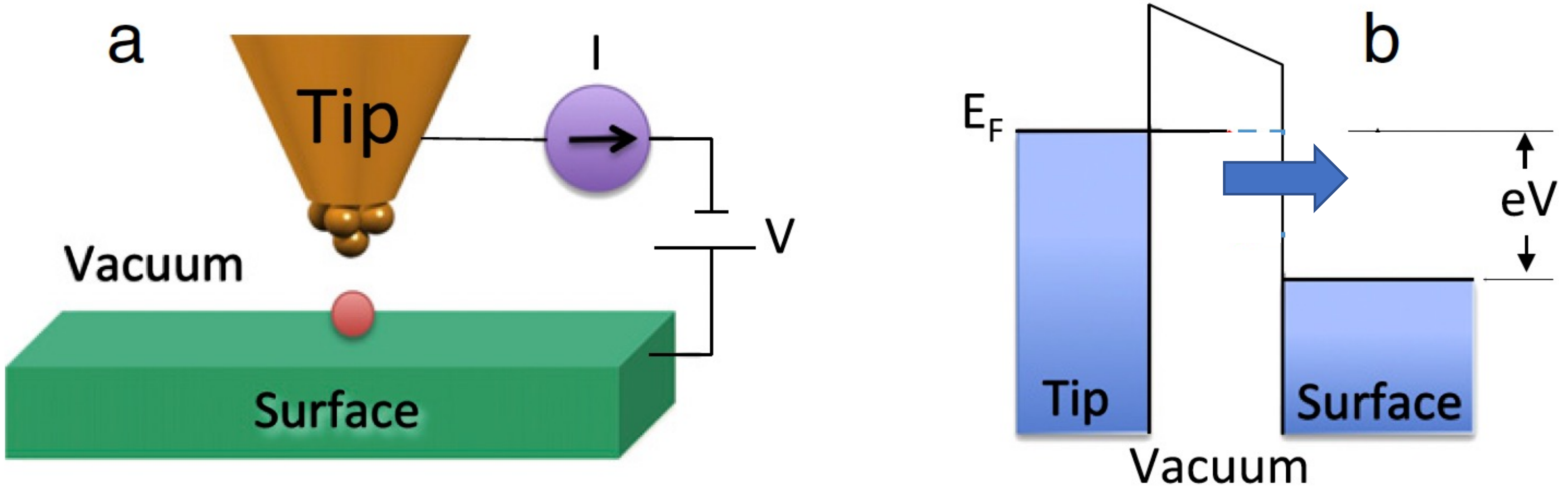
$$\psi(z) = \psi(0)e^{-\kappa z}$$

with $\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

in particular $\psi(d) = \psi(0)e^{-\kappa d}$

→ tunneling probability $\propto |\psi(d)|^2 = |\psi(0)|^2 e^{-2\kappa d}$

Scanning tunneling microscopy (STM)



tunneling current:
$(k_B T \ll eV)$

$$I \propto \int_0^{eV} \rho_t(E_F - eV + \varepsilon)\, \rho_s(E_F + \varepsilon) |M(\varepsilon)|^2 d\varepsilon$$

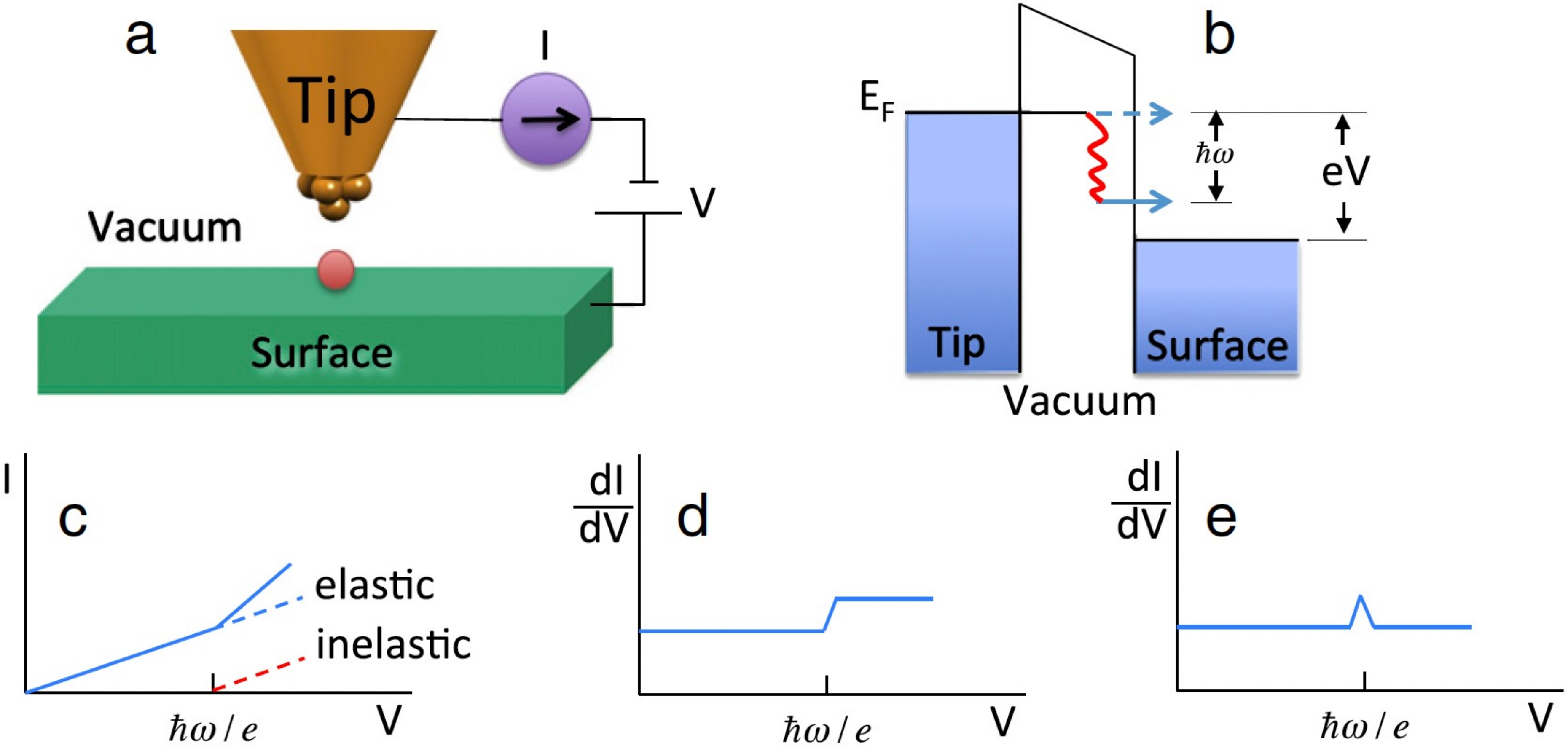
tip density of states

sample density of states

tunneling probability
$\propto \exp(-2\kappa d)$

figure adapted from http://dx.doi.org/10.1016/j.susc.2014.07.014

Inelastic electron tunneling spectroscopy (IETS)

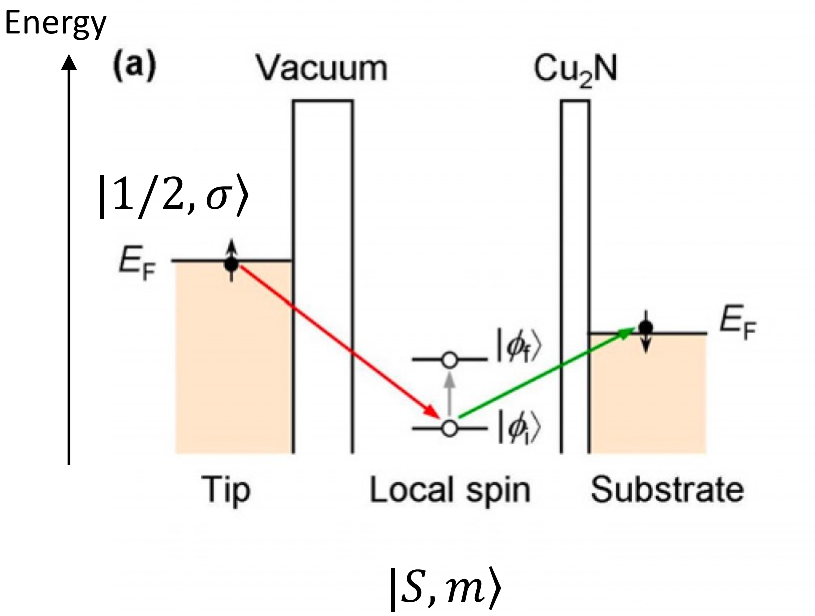


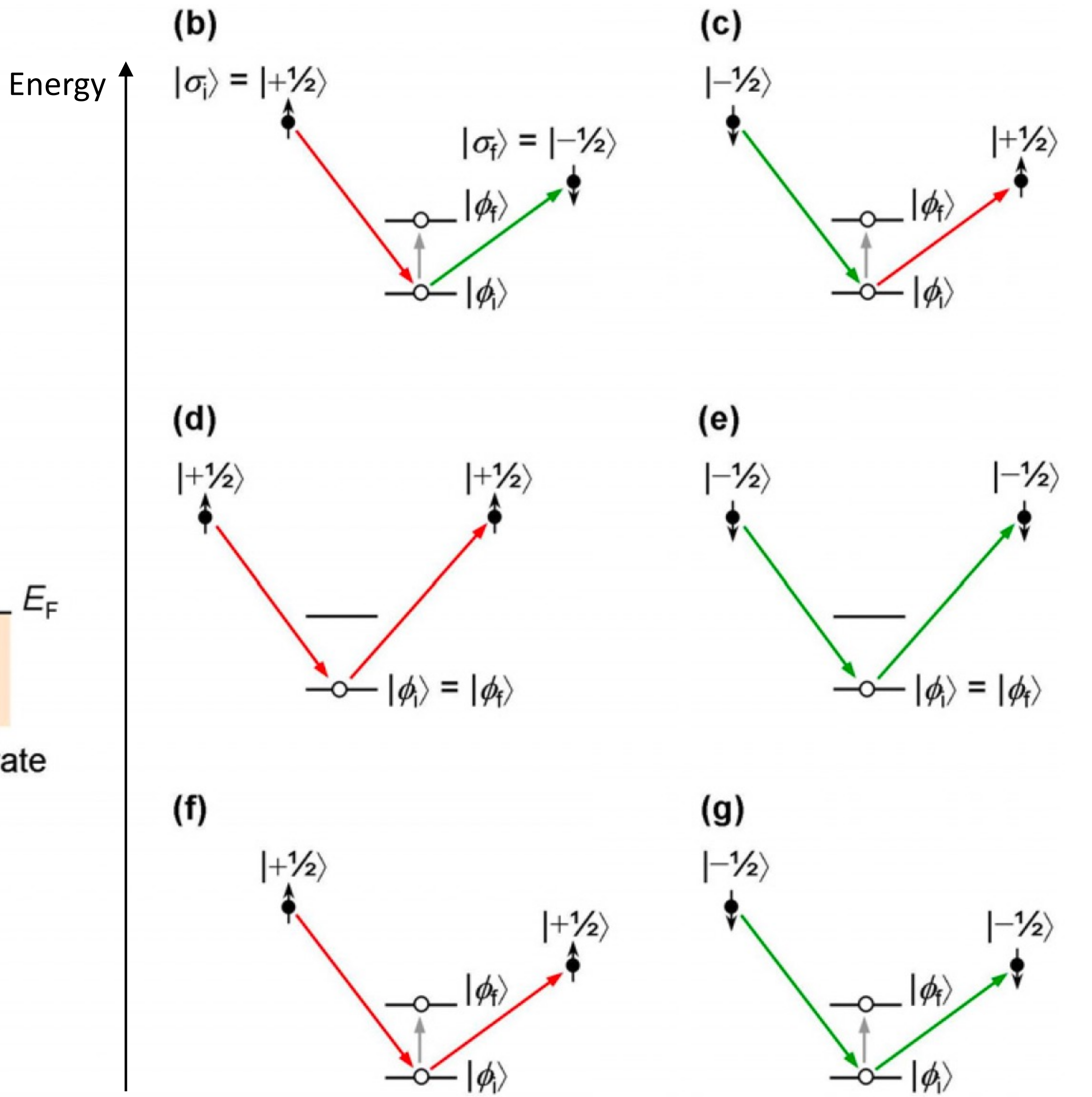
Consider an object at the surface (molecule, adatom, nanostructure...).
The tunneling electrons trigger an excitation of the adsorbate (vibration, rotation, spin flip, magnetic excitation...): they couple to the excitation mode and loose part of their energy; an additional tunneling channel is created.
This results in an increase of the tunneling current with respect to the elastic channel.

An inelastic tunneling channel opens, at a specific energy, in addition to the elastic one. The inelastic feature is present in both bias polarities.

IETS: spin excitations

hamiltonian for s-e scattering: $J_{exc}\, S_z \sigma_z + 1/2\, J_{exc}\, (S_+ \sigma_- + S_- \sigma_+)$





$\Delta\sigma = \mp 1$
$\Delta m = \pm 1$
$\Delta E \neq 0$

$\Delta\sigma = 0$
$\Delta m = 0$
$\Delta E = 0$

$\Delta\sigma = 0$
$\Delta m = 0$
$\Delta E \neq 0$

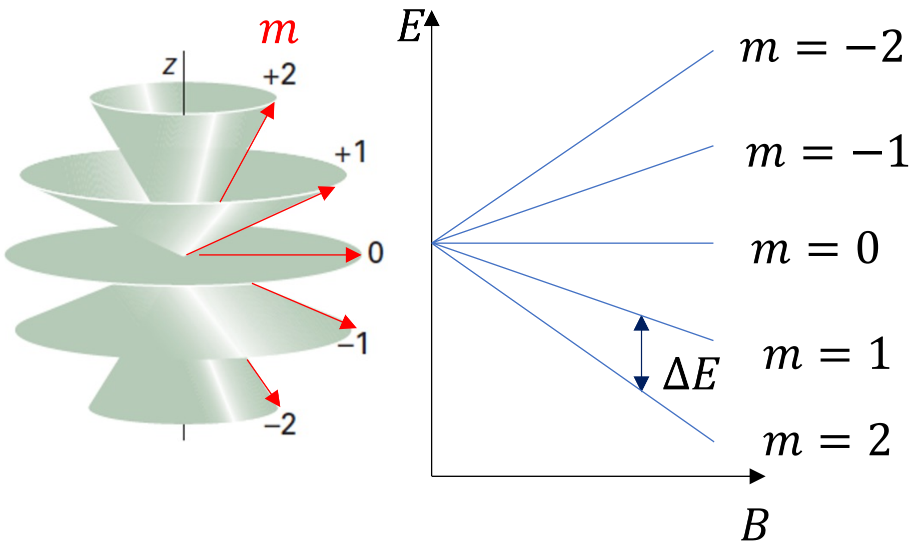
Loth et al., New J. Phys. **12** 125021 (2010)

IETS: spin excitations

Zeeman energy for a paramagnetic spin $|S, m\rangle$
(magnetic moment $\boldsymbol{\mu} = -g\mu_B \boldsymbol{S}$)

example:

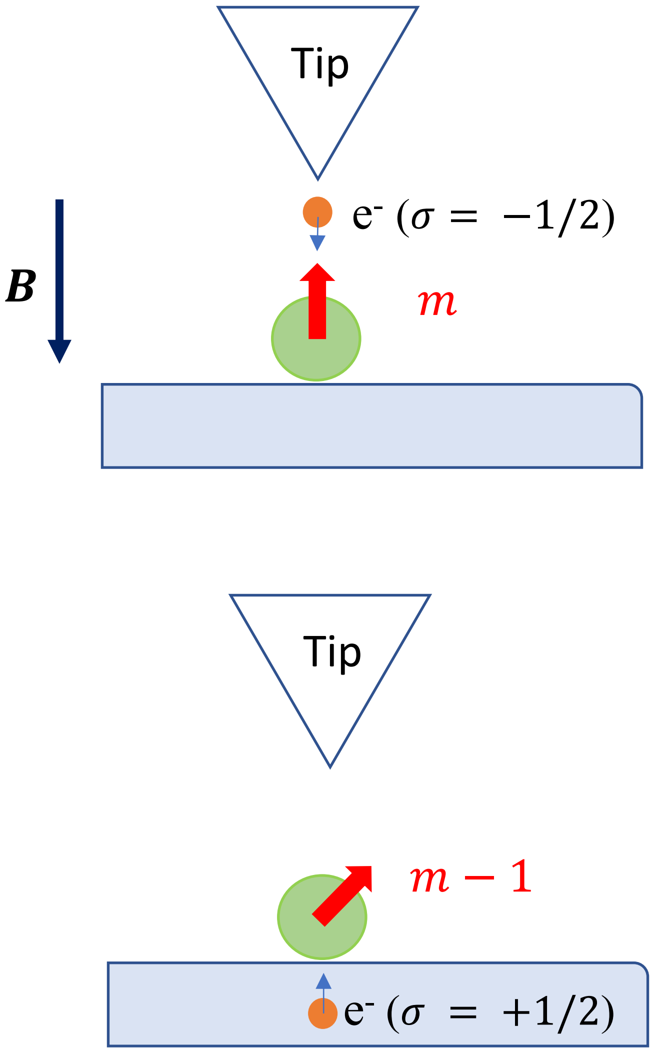
$S = 2; \quad m = -2, .., 2$



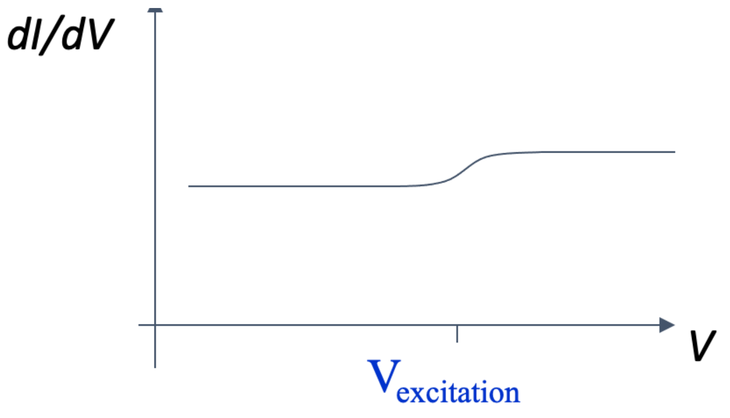
$H_{Zee} = g\mu_B \boldsymbol{S} \cdot \boldsymbol{B}$

$E(m) = g\, \mu_B m\, B$

$\Delta E = |g\mu_B B\, \Delta m|$



we expect:



$eV_{excit} = g\mu_B B$

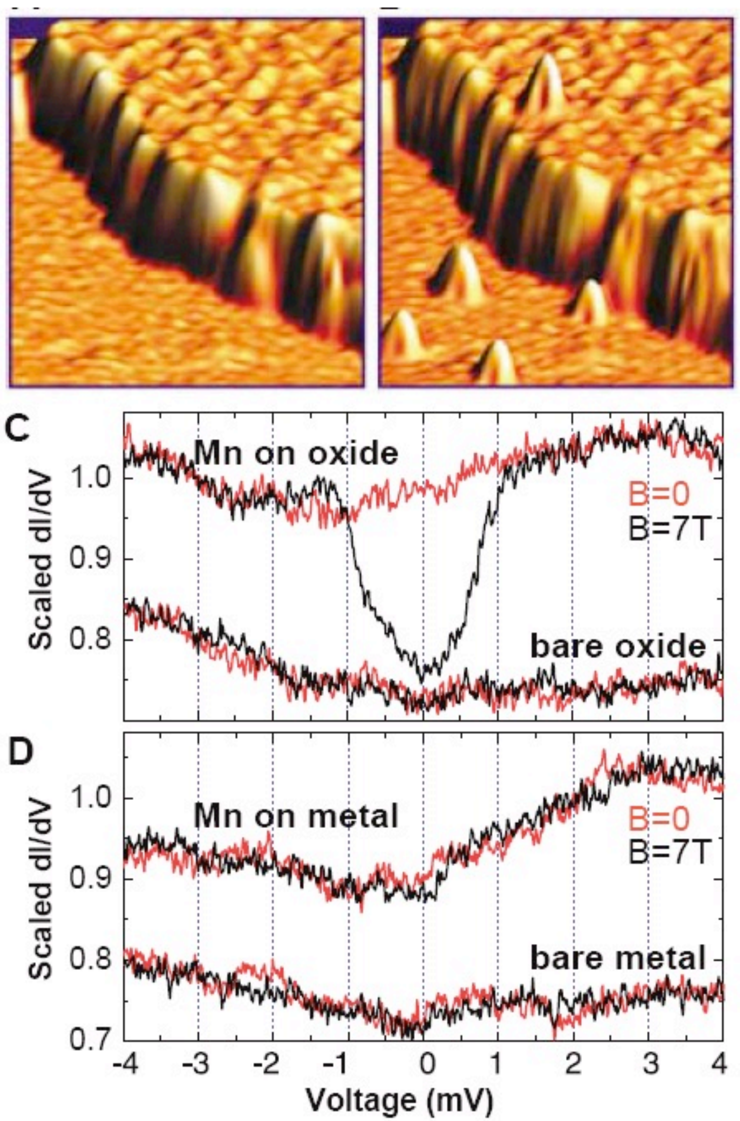
$\Delta\sigma = +1 \rightarrow \Delta m = -1$

$\Delta E = |g\mu_B B|$

An inelastic tunneling process can involve energy and momentum transfer from the tunneling electron to the atom spin which flips from the ground to an excited state.

Example: Mn/Al_2O_3

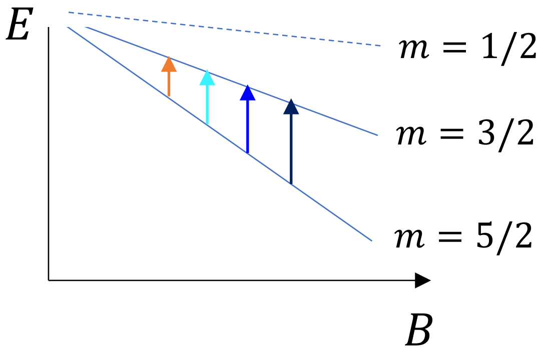
$Mn/Al_2O_3/Ni_3Al(111)$



Heinrich et al., Science 2004 10.1126/science.1101077

free Mn atom: [Ar]$3d^5$ $4s^2$

$$S = \frac{5}{2}, L = 0$$



$$eV_{excit} = g\mu_B B$$

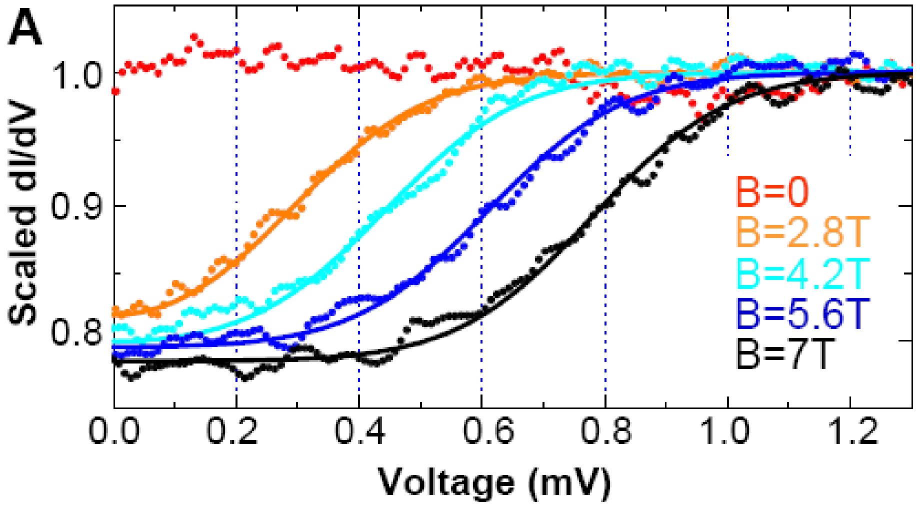
$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

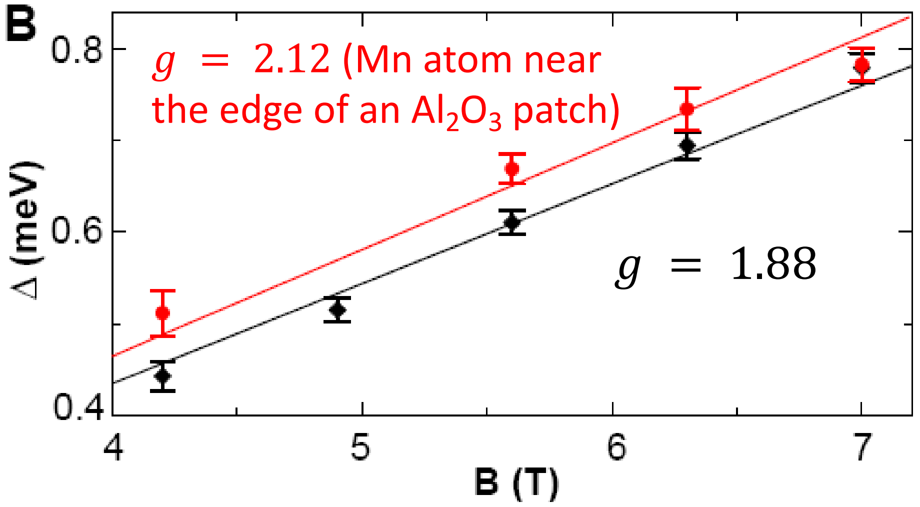
g is the Landé g-factor.

For $L = 0 \rightarrow g = 2$

T = 0.6 K

Shift of the spin-flip conductance step with magnetic field



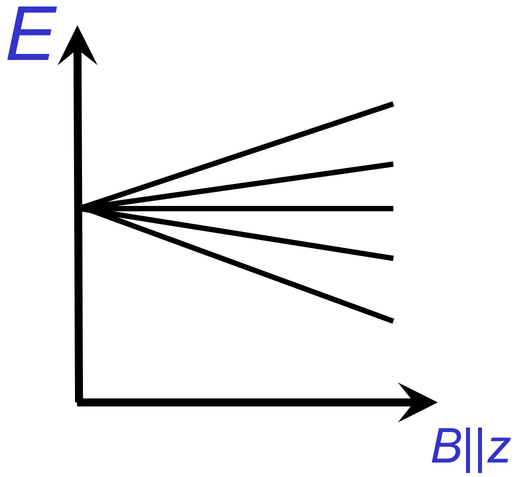


weak influence of the crystal field (local environment)

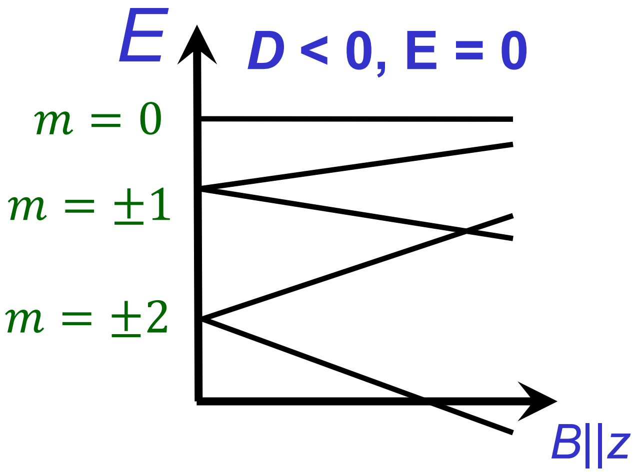
Crystal field: Effect of *D* and *E* parameters (C_{2v})

Energy spectrum: example for $S = 2$

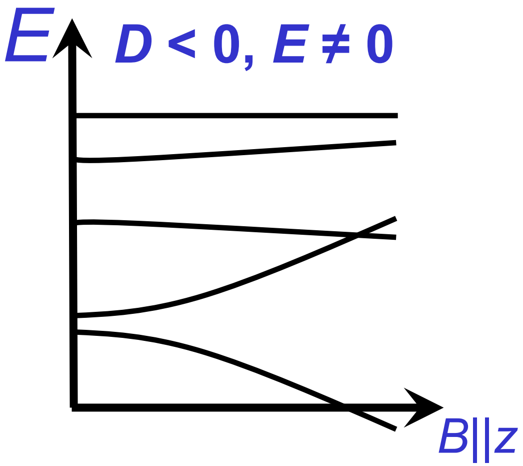
CF = 0



axial CF

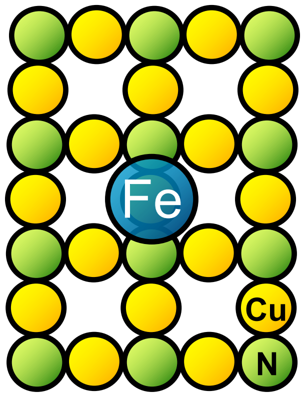


distorted (C_{2v}) CF



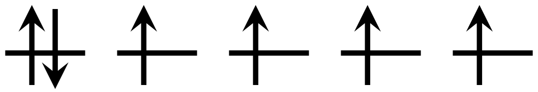
$$H_{eff} = g_z \mu_B (H_z S_z) + D S_z^2 + E(S_x^2 - S_y^2)$$

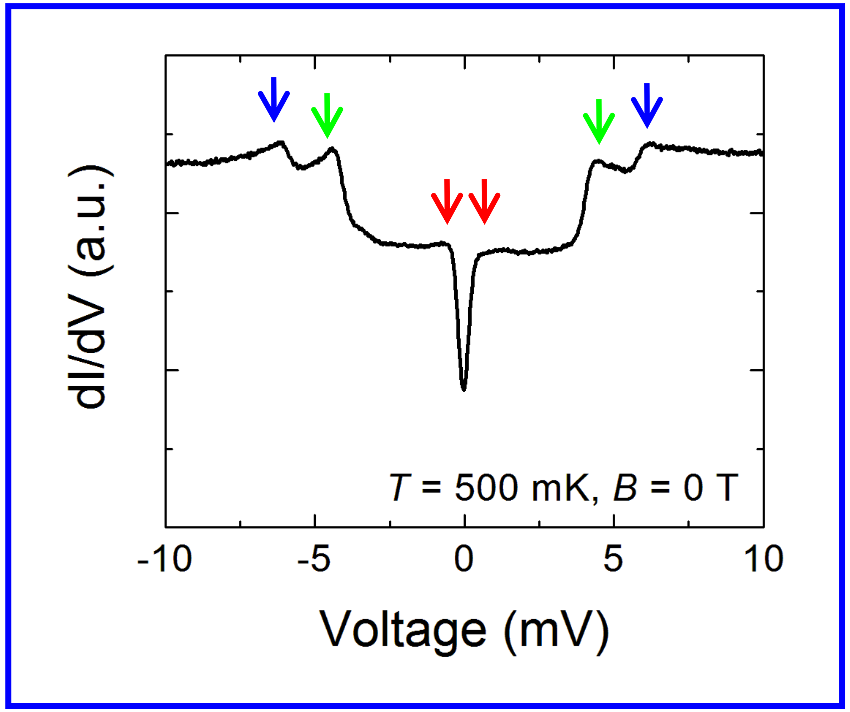
Example: $Fe/Cu_2N/Cu(001)$



free Fe atom: [Ar] $3d^6\ 4s^2$

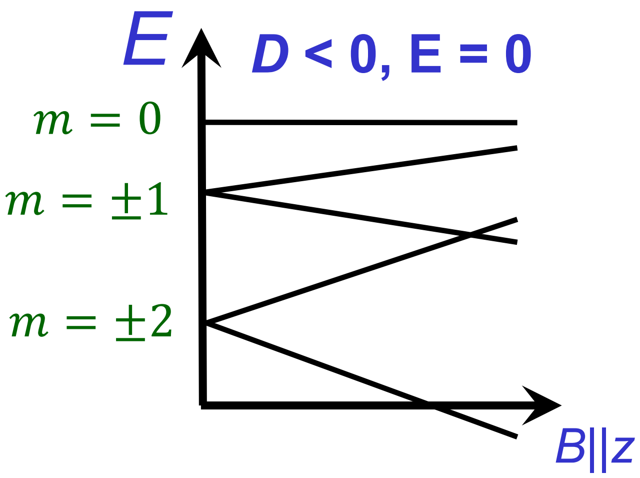
$S = 2, L = 2$

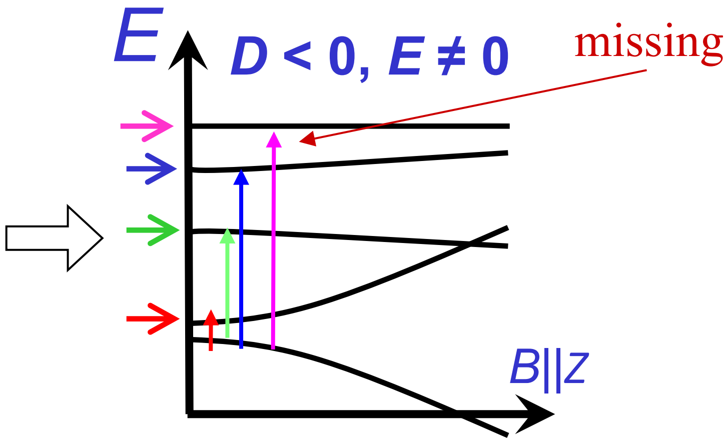




$$H_{eff} = g\mu_B S_z B + DS_z^2 + E\left(S_x^2 - S_y^2\right)$$

z is in the plane, along the N-row (magnetization easy axis)





Hirjibehedin *et al.*, Science **317**, 1199 (2007)

Example: $Fe/Cu_2N/Cu(001)$

Eigenstates $|\Psi_i\rangle$ and eigenvalues E_i of H for a given field B

Eigenstate		$\|+2\rangle$	$\|+1\rangle$	$\|+0\rangle$	$\|-1\rangle$	$\|-2\rangle$	Eigenvalues
				B = 0 T			
ψ_0	σ_z	0.697	0	−0.166	0	0.697	0 meV
ψ_1		0.707	0	0	0	−0.707	0.18 meV
ψ_2	σ_-,σ_+	0	0.707	0	−0.707	0	3.90 meV
ψ_3		0	0.707	0	0.707	0	5.76 meV
ψ_4		0.117	0	0.986	0	0.117	6.56 meV
				B = 7 T			
ψ_0		0.021	0	−0.097	0	0.995	
ψ_1		0.987	0	−0.157	0	−0.036	
ψ_2		0	0.402	0	−0.916	0	
ψ_3		0	0.916	0	0.402	0	
ψ_4		0.159	0	0.983	0	0.092	

$S = 2,\ g = 2.11,\ D = -1.55$ meV, $E = 0.31$ meV

S integer, $E \neq 0$ → quantum tunneling: at $B = 0$ the ground state Ψ_0 (and Ψ_1) is a superposition of $|+2\rangle$ and $|-2\rangle$ → $\langle S_z\rangle = 0$

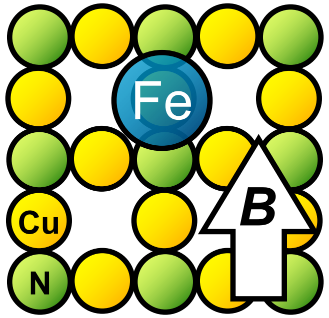
B splits the states (i.e. the states are almost pure) and restore a moment: at $B = 7$ T → $\langle S_z\rangle = \pm 2$

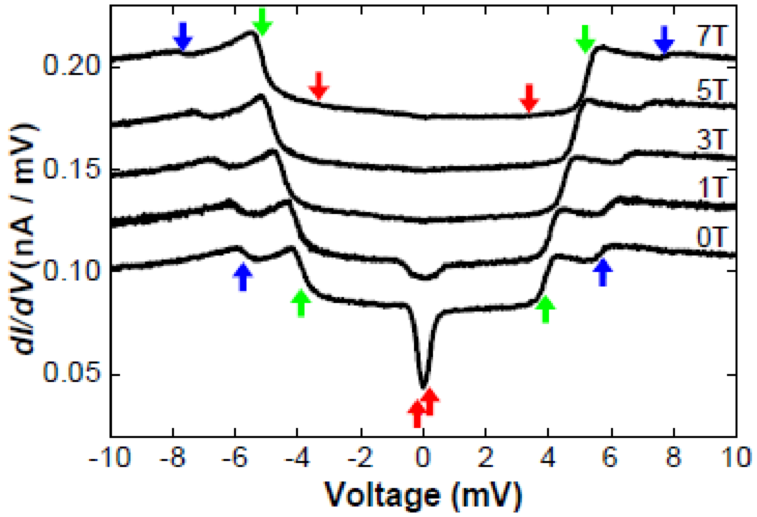
$T_1 \sim h/(\Delta E) = 200$ ns ($B = 0$ T) → very short spin lifetime

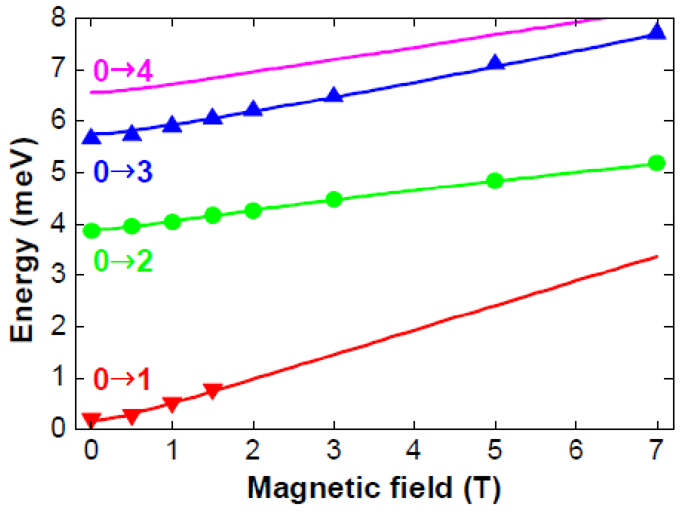
Hirjibehedin *et al.*, Science **317**, 1199 (2007)

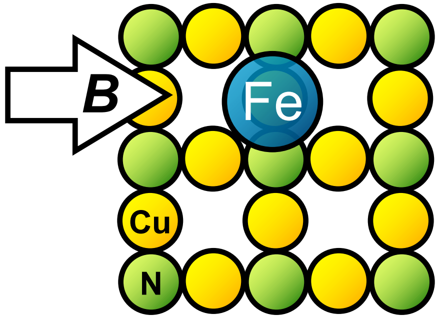
Example: Fe/Cu_2N/Cu(001)

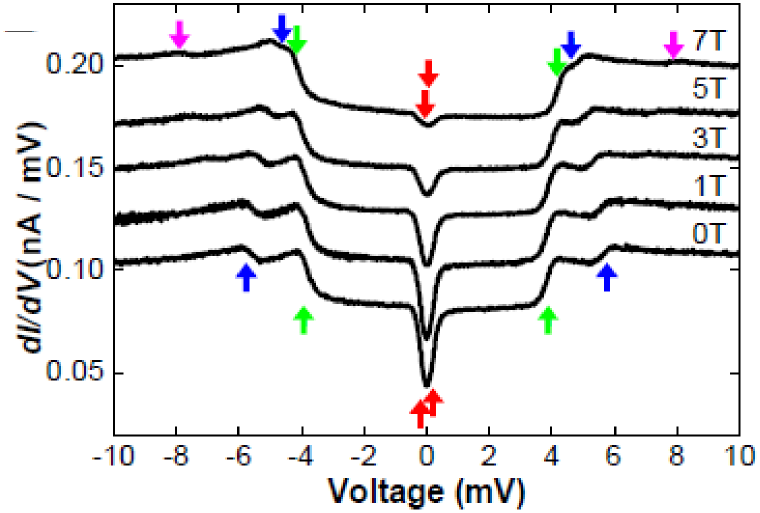
Spectra depend on B field direction → magnetic anisotropy

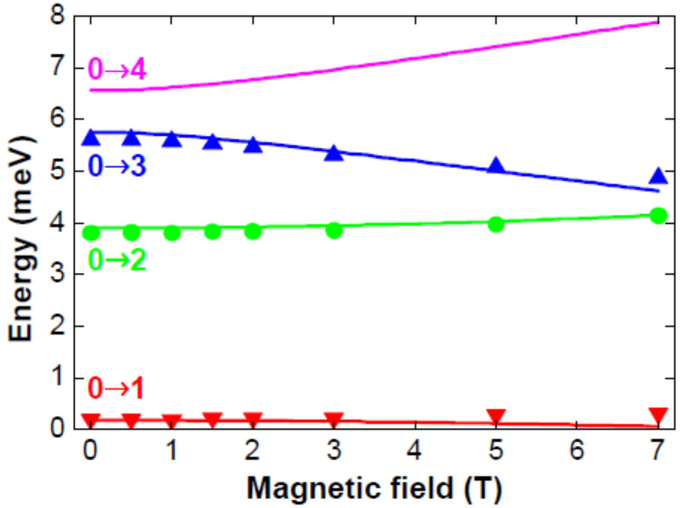






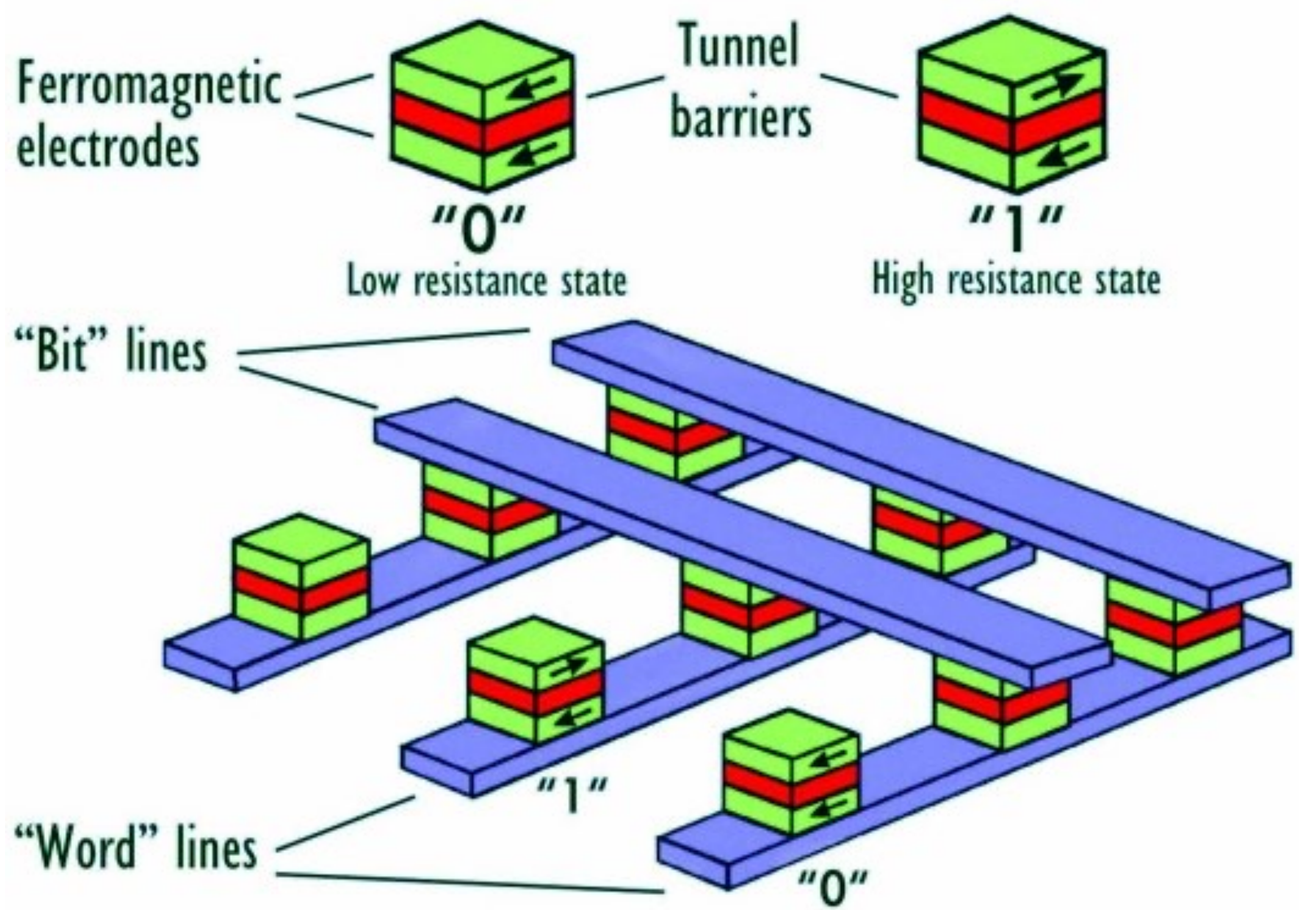






Hirjibehedin *et al.*, Science **317**, 1199 (2007)

MRAM: downscaling to single atom?

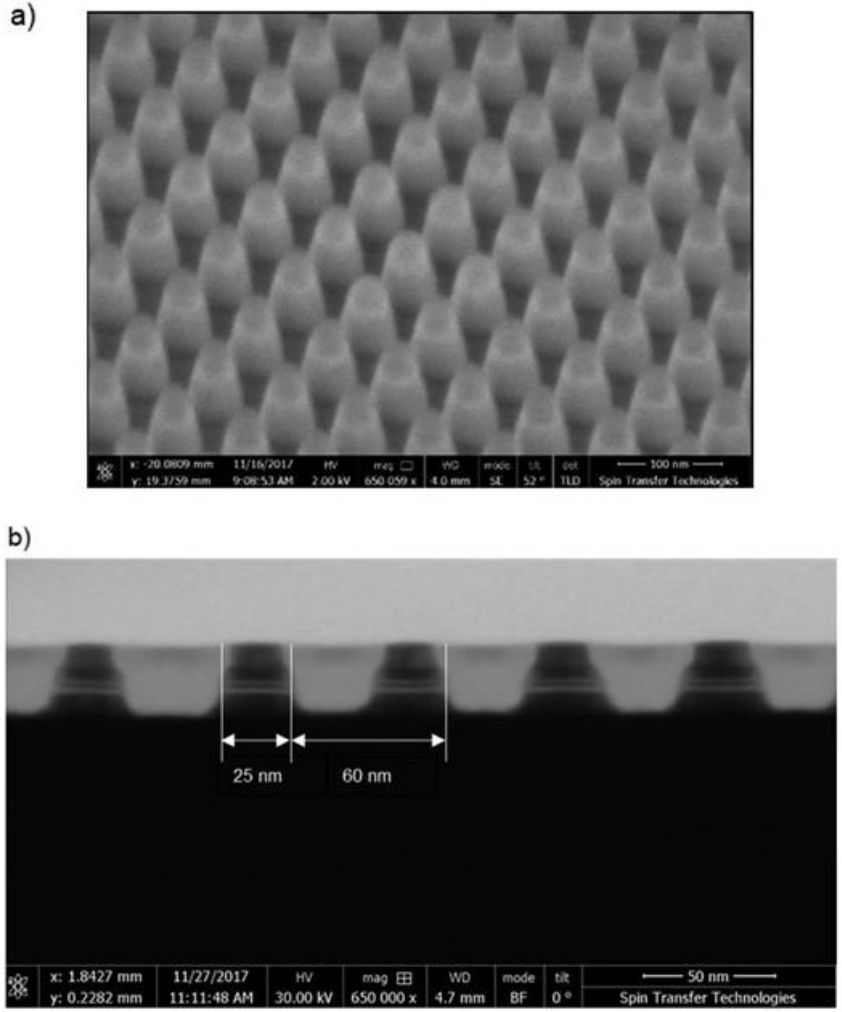


Reading: by measuring the point contact resistance between a bit and a word line

Writing: by magnetic fields (toggle-MRAM) or by injecting spin polarized current i.e. spin transfer torque (STT-MRAM) through the point contact

a)

b)



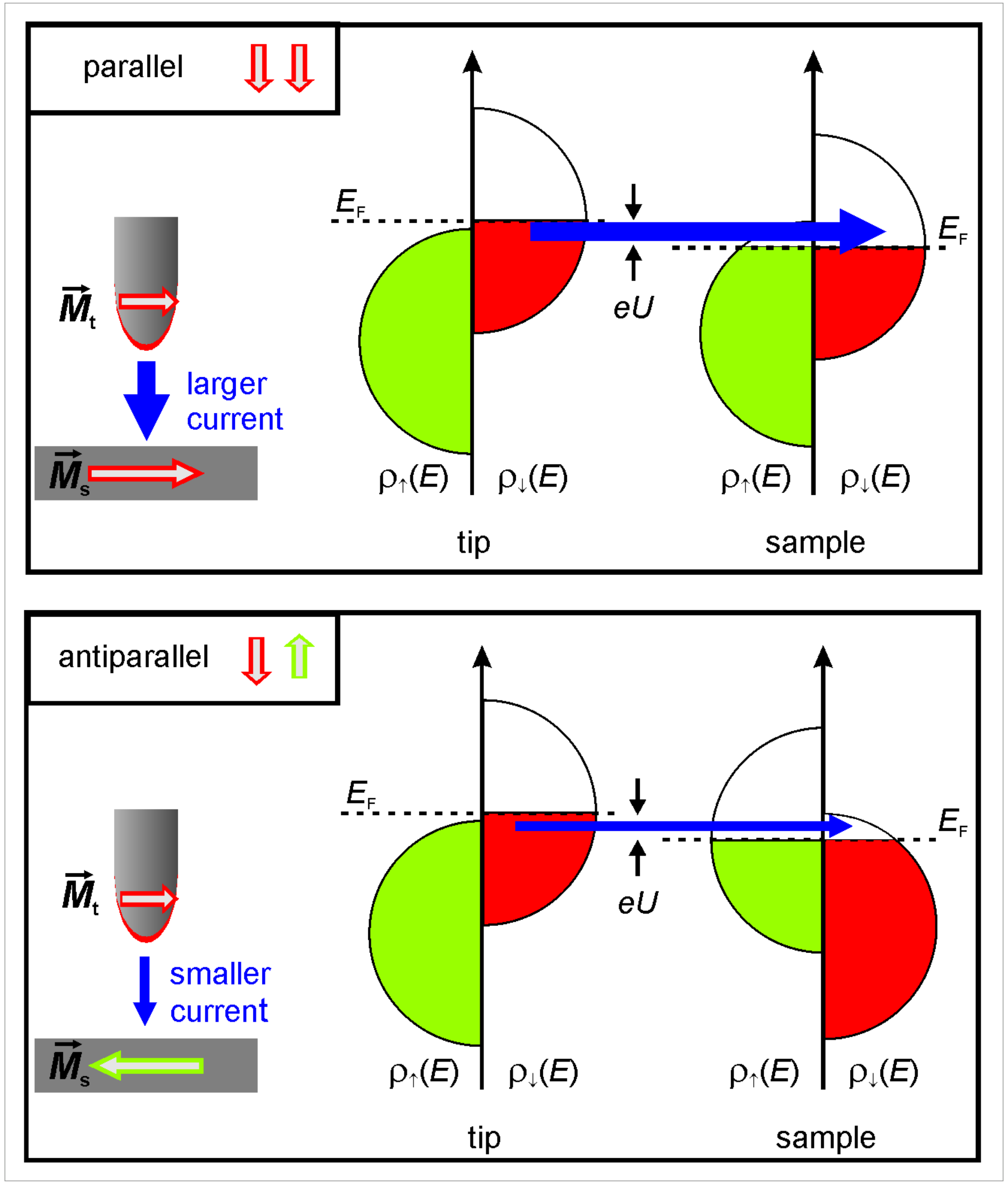
VIEW LARGE DOWNLOAD SLIDE

(a) SEM picture shows the wafer surface for high density processing at an intermediate processing step. The pillar structures are shown after photoresist and reactive ion etching of the hard mask layer. The hard mask layer protects the pMTJ structure during the ion beam etching. (b) The cross section of the high density pillars after they are formed. The pillar diameters are ~25 nm with ~60 nm pitch, demonstrating capabilities to make high density chips.

Science **282**, 1660 (1998); Nat. mater. **6**, 813 (2007)

https://doi.org/10.1063/5.0075945

Spin-polarized STM



The tunneling current is the sum of two contributions

$$I \propto I^{\uparrow} + I^{\downarrow}$$

At fixed bias and tip-sample distance, the tunneling current changes depending on the alignment of tip and sample magnetization

Junction spin polarization:
(magnetoresistance)

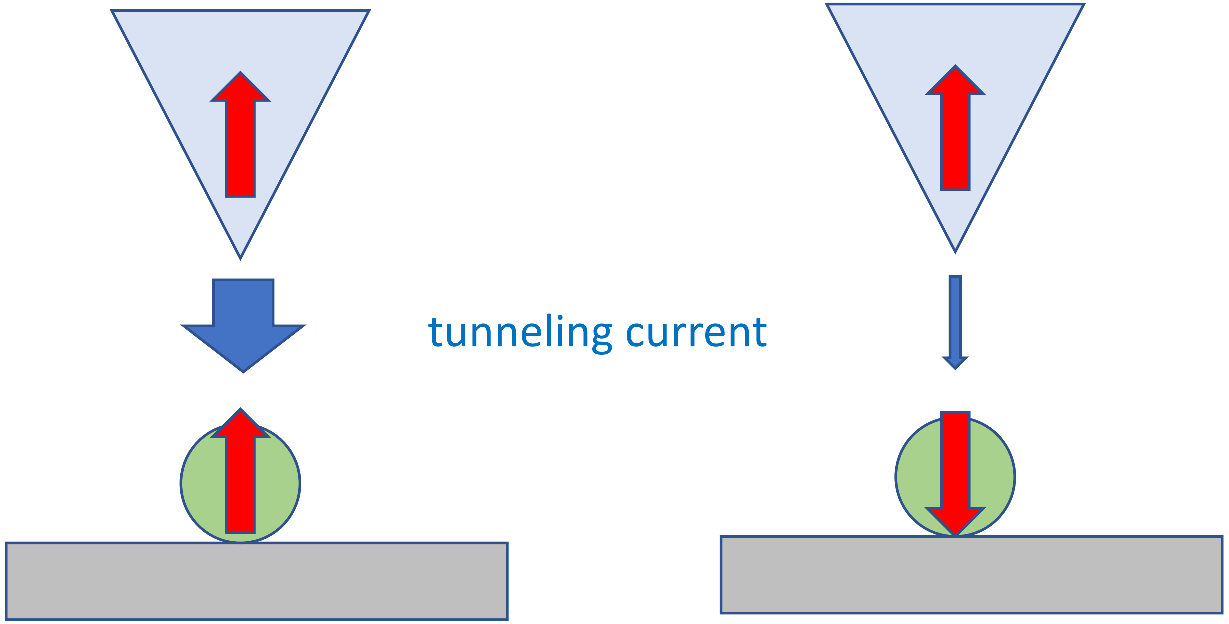
$$P = \frac{I^{high} - I^{low}}{I^{high} + I^{low}}$$

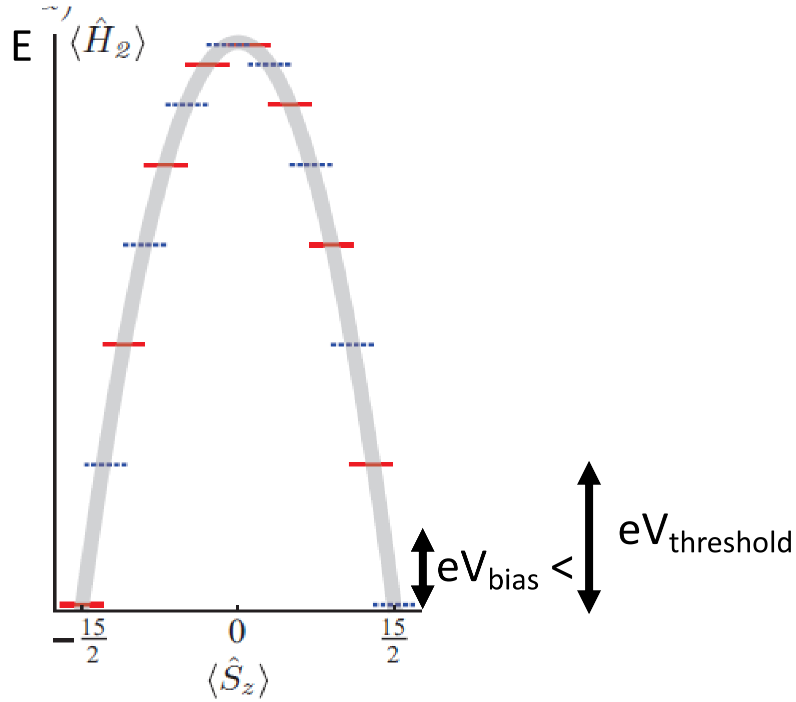
$$P \sim P_{tip}\, P_{sample}\, \cos\theta$$

determination of the orientation (θ) of the sample magnetization with respect to the one of the tip

R. Wiesendanger group
http://www.nanoscience.de/HTML/methods/sp-stm.html

Spin-polarized STM: reading the spin state of a single atom



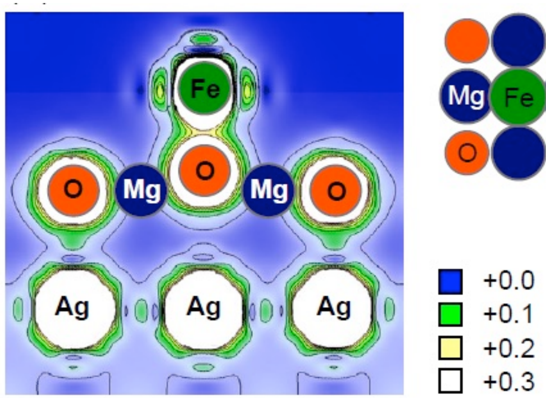


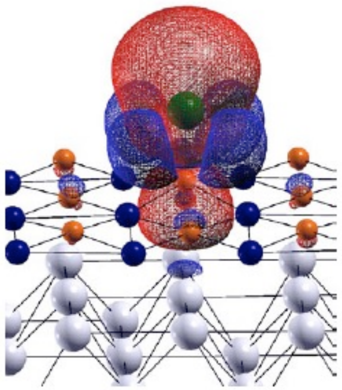
at constant height high current low current

measurement vs. time:

- a change in the orientation of the atom magnetization is detected as a change in current (telegraph signal, magnetic contrast)
- determination of the spin lifetime

Example C_{4v}: Fe/MgO/Ag(100)





free Fe atom: [Ar]$3d^6\ 4s^2$

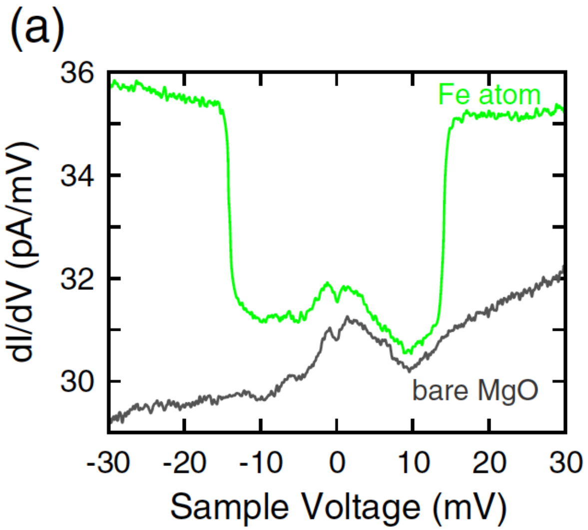
$$S = 2, L = 2$$

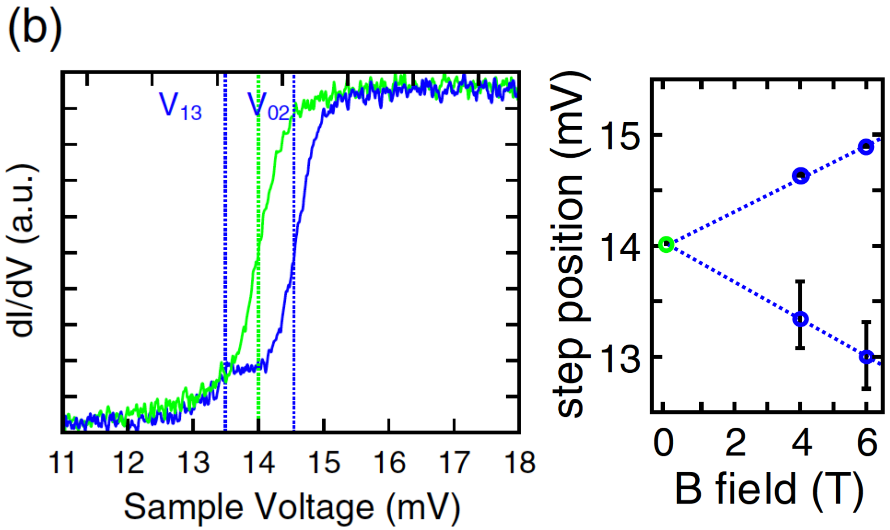
$$H_{eff} = g\mu_B S_z B + DS_z^2 + C(S_-^4 + S_+^4)$$

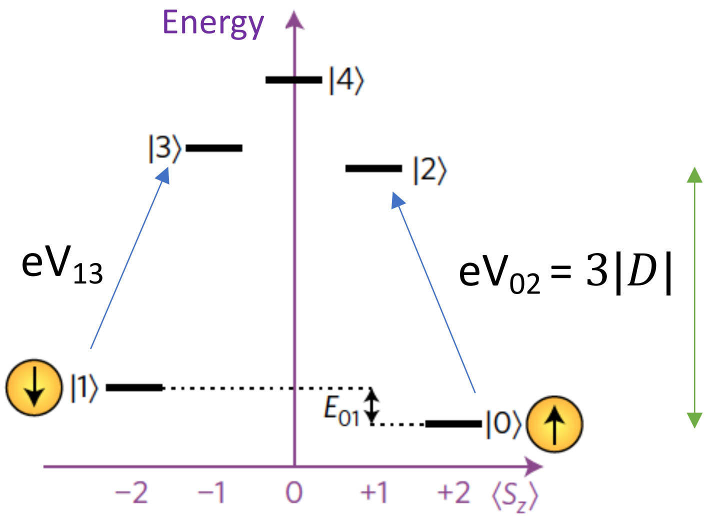
z is perpendicular to the surface

$D = -4.7$ meV, $C = 41$ neV, $g = 2.6$

ground and first excited state $|0\rangle, |1\rangle$: $\langle S_z \rangle \approx \pm 2$



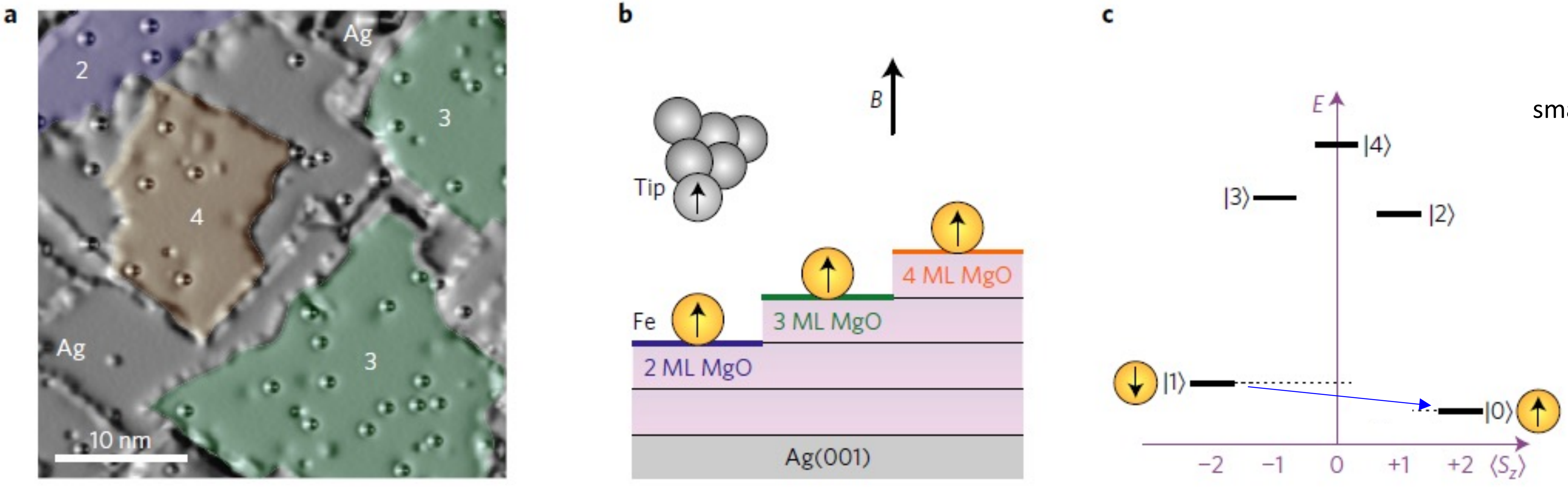




The zero-field splitting between state 0 and state 1 due to the transverse term C is too small to be detected at $T = 0.6$ K

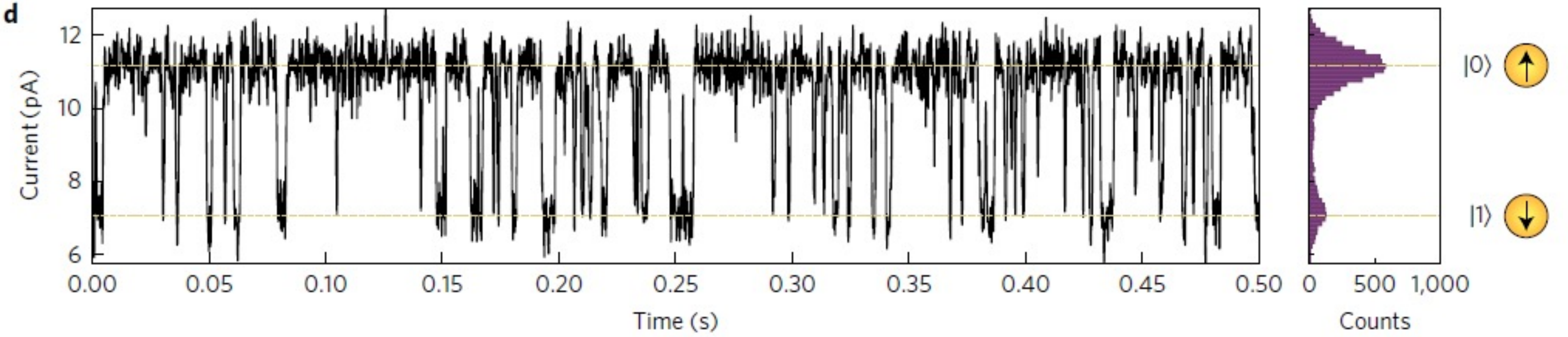
S. Baumann *et al.* Phys. Rev. Lett. **115**, 237202 (2015), W. Paul *et al.*, Nat. Phys. **13**, 403 (2017)

Fe/MgO/Ag(100): telegraph signal



small but finite overlap →
$(\langle 0|S_z|1\rangle)^2 \neq 0$

Telegraph signal



$T = 1.2$ K

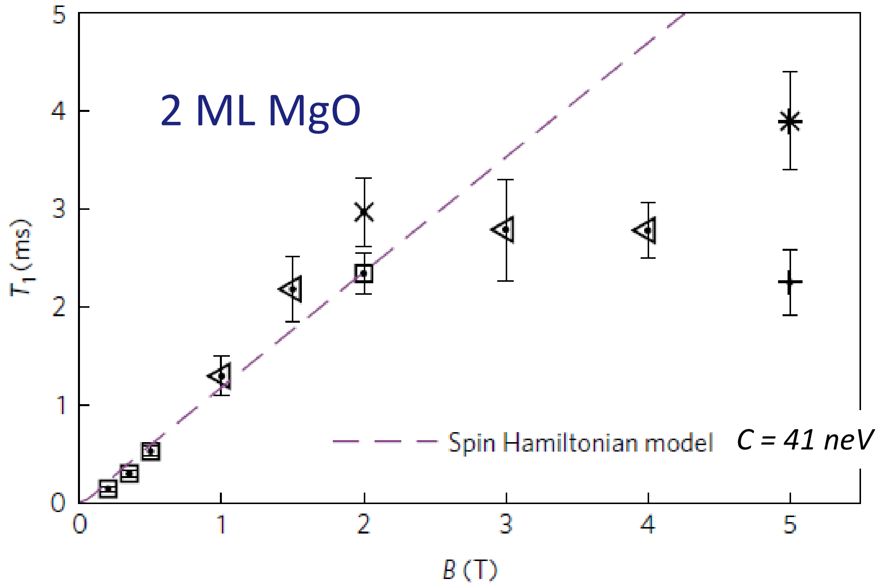
$B = 2.5$ T

$V_{bias} = 10$ mV

lifetime T_1 = (switching rate)$^{-1}$

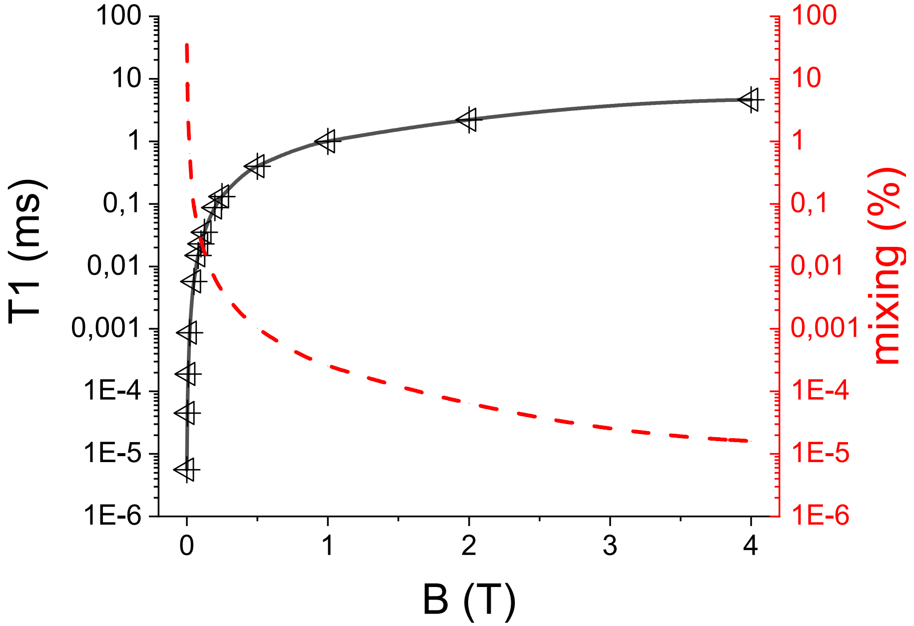
W. Paul *et al.*, Nat. Phys. **13**, 403 (2017)

Fe/MgO/Ag(100): spin lifetime

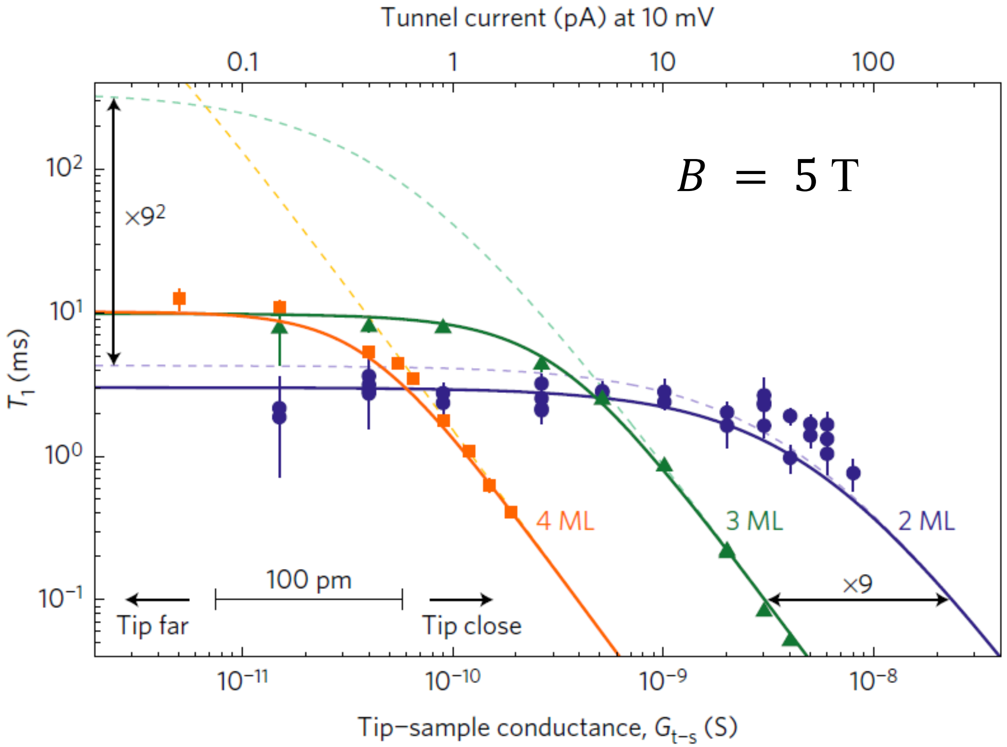


Due to the C_{4v} CF, $|0\rangle$ and $|1\rangle$ are not pure states → QTM → $T_1 = 0$ at $B = 0$ T

The external field B restores the pure spin states → no QTM → longer T_1



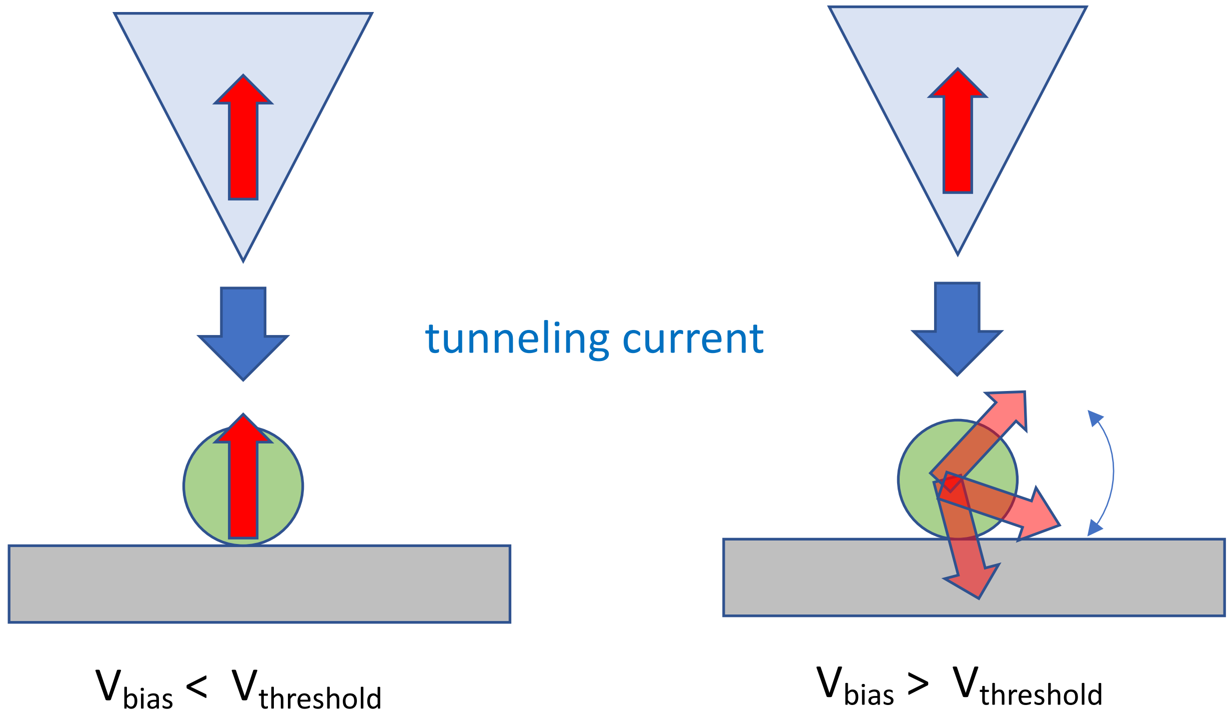
Increasing the MgO thickness, T_1 increases due to reduced scattering with the electrons of the supporting Ag(100) crystal

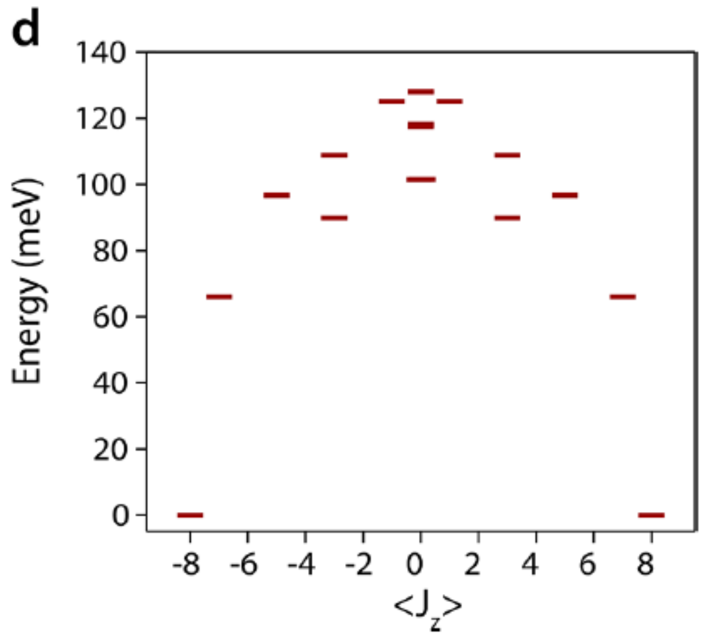


STT at the single atom scale: writing the spin state

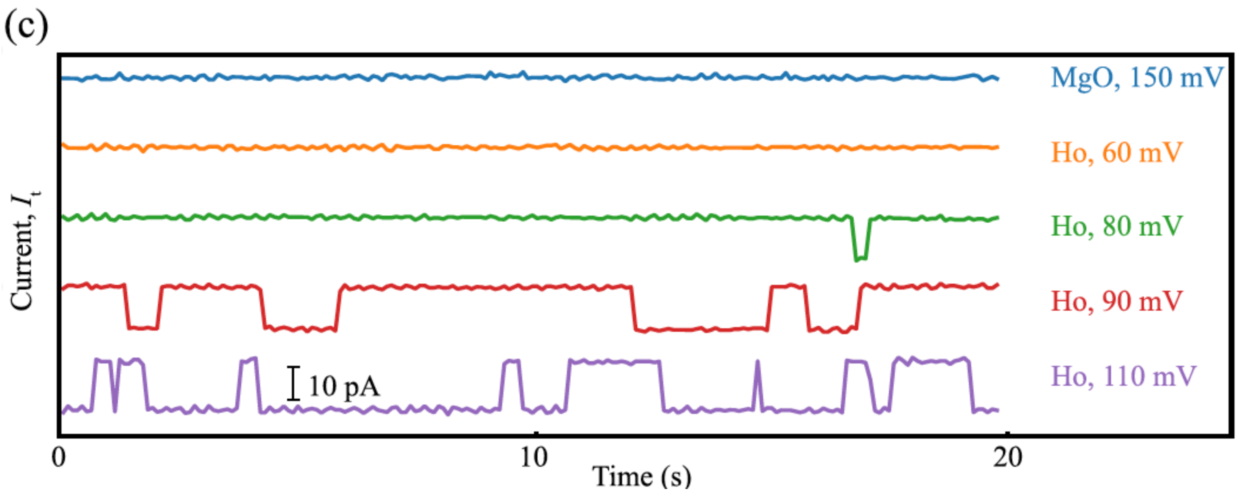
See exercise: 9.1

Ho / MgO / Ag(100)

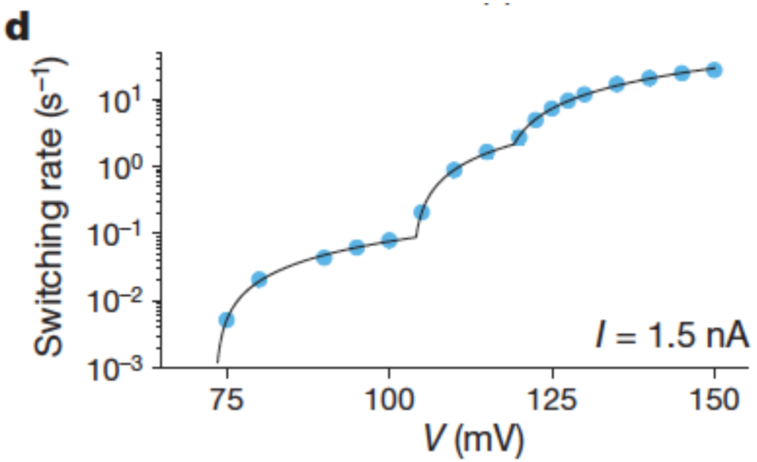




$4f^{10}$:
S=2
L=6
J=8

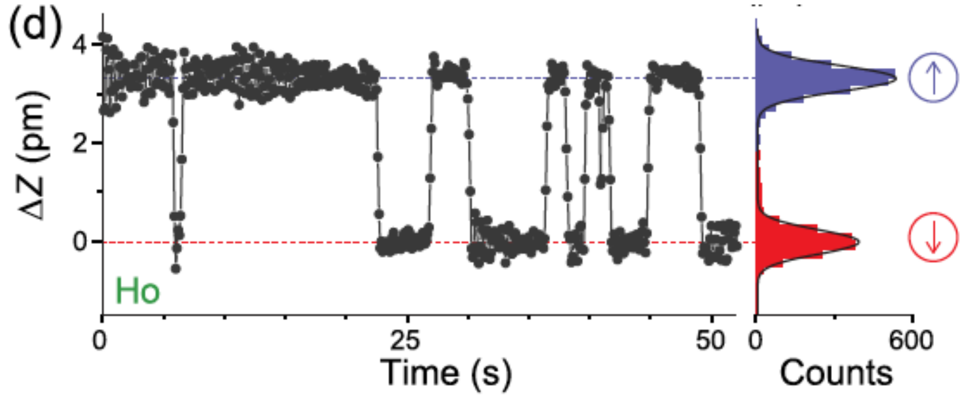


T = 4.7 K
I =100 pA
B ~10 mT
(tip stray field)



Natterer *et al.,* Nature **543**, 226 (2017); Natterer *et al.,* Phys. Rev. Lett. **121**, 027201 (2018); Forrester et al., Rev. Sci. Instrum. **89**, 123706 (2018)

STT at the single atom scale: writing the spin state



T = 4.3 K

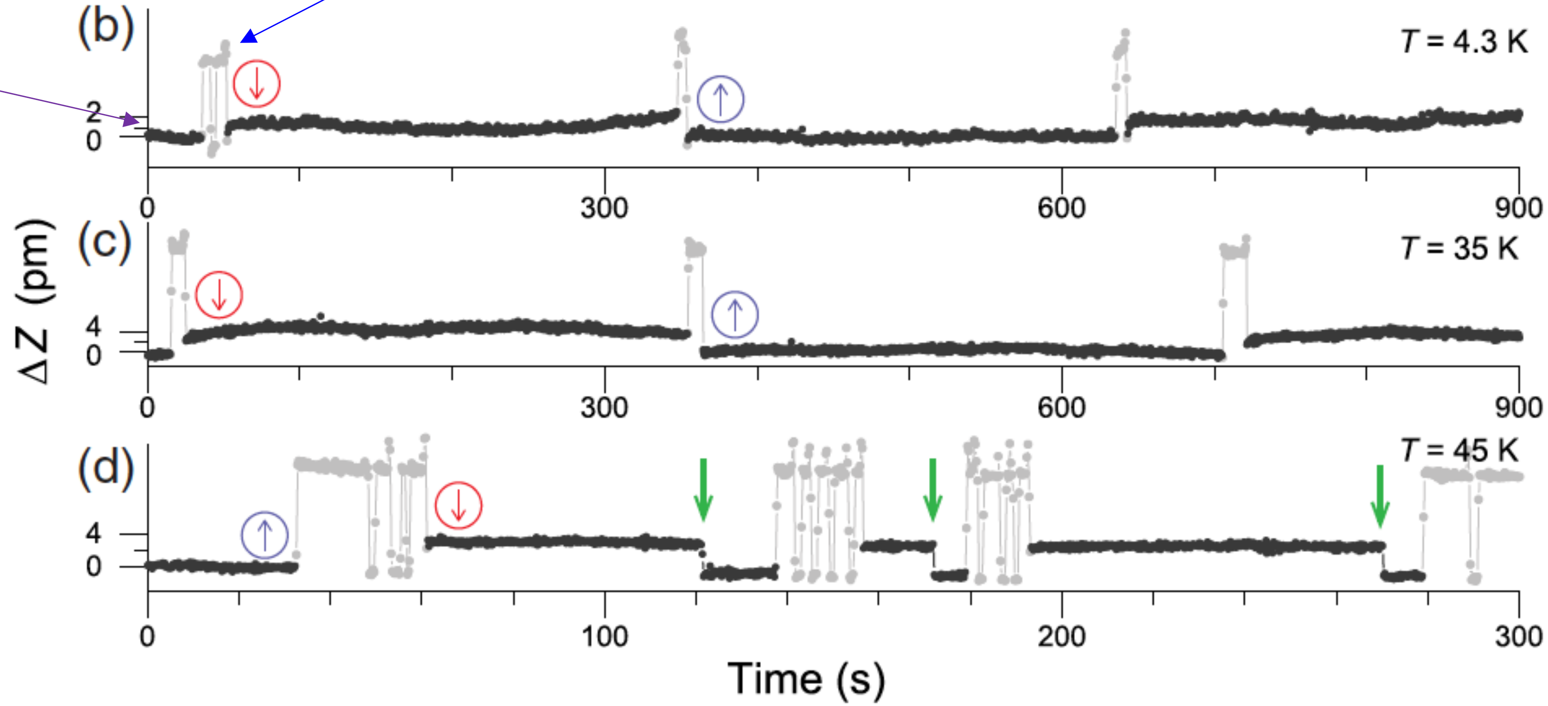
B = 4 T

V_{bias} = 150 mV

Ho / MgO / Ag(100)

current pulse at V_{bias} = 150 mV to write the spin state

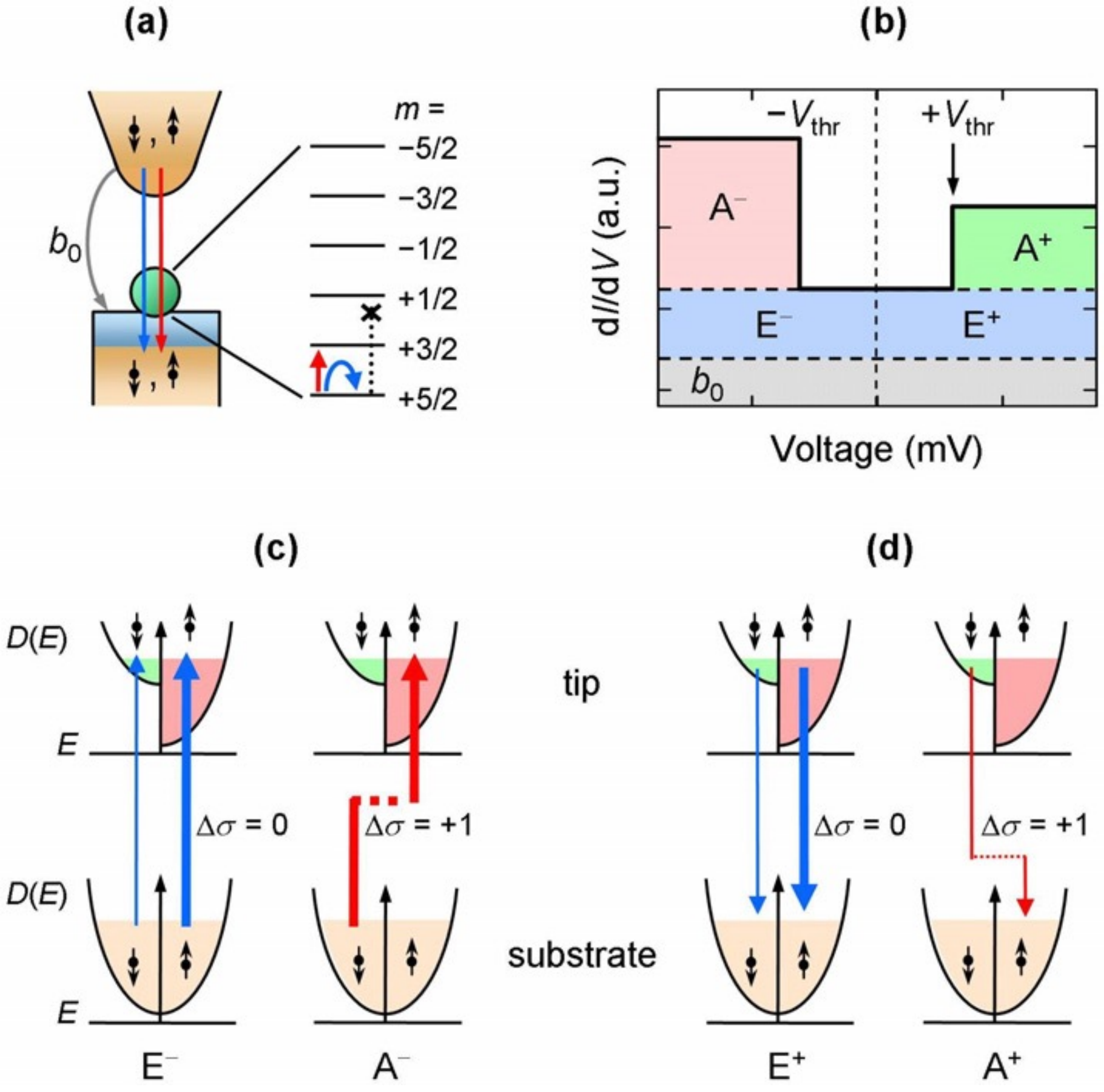
V_{bias} = 50 mV to read (monitor) the spin state



at T = 45 K spontaneous switching starts to appear

Natterer et al. Phys. Rev. Lett. **121**, 027201 (2018)

$|S, m\rangle$



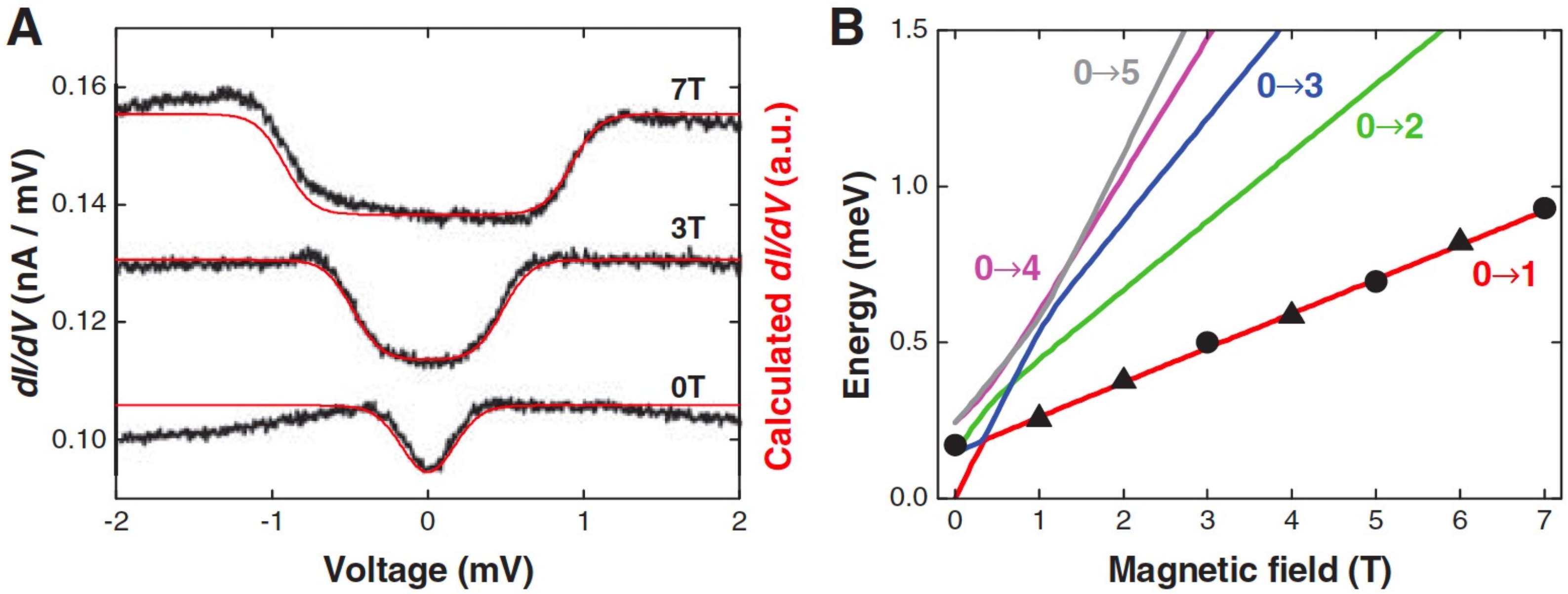
free Mn atom: [Ar]3d^5 4s^2

$$S = \frac{5}{2}, L = 0$$

$$\Delta\sigma = +1$$
$$\Delta m = -1$$
$$\Delta E \neq 0$$

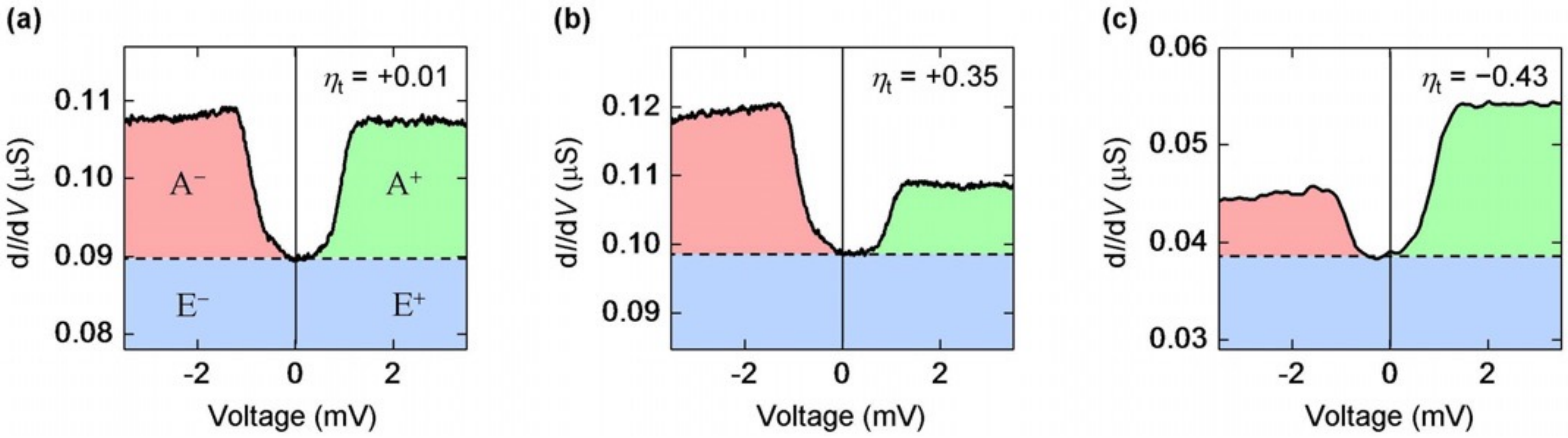
Loth et al., New J. Phys. **12** 125021 (2010)

Example: $Mn/Cu_2N/Cu(100)$



easy axis oriented out-of-plane

$$g = 1.90$$
$$D = -0.039 \text{ meV}$$
$$E = 0.007 \text{ meV}$$

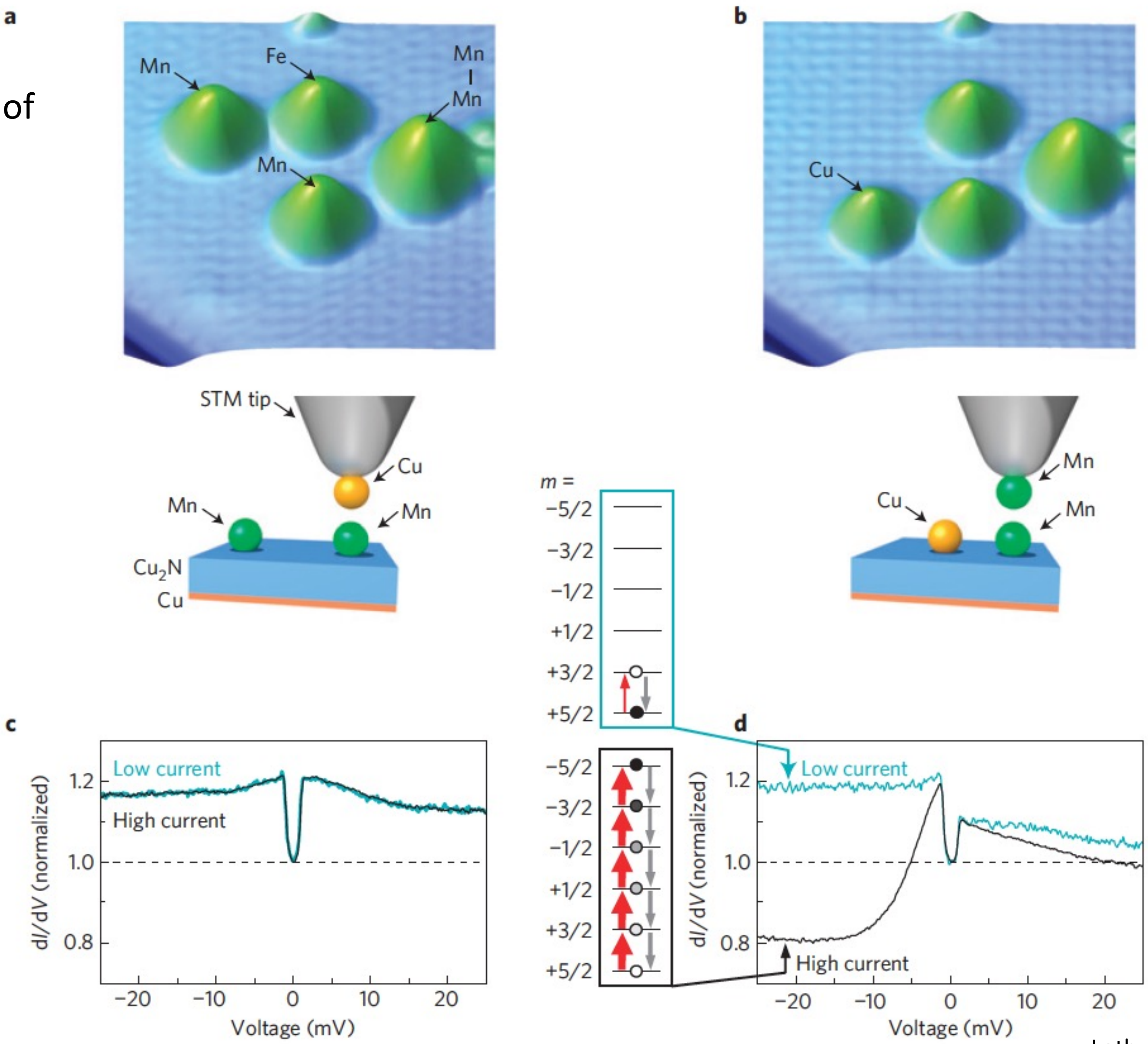


Hirjibehedin *et al.*, Science **317**, 1199 (2007); Loth et al., New J. Phys. 12 125021 (2010)

Example: Mn/Cu_2N/Cu(100)

See exercise: 9.2

Controlling the state of quantum spins with electric currents

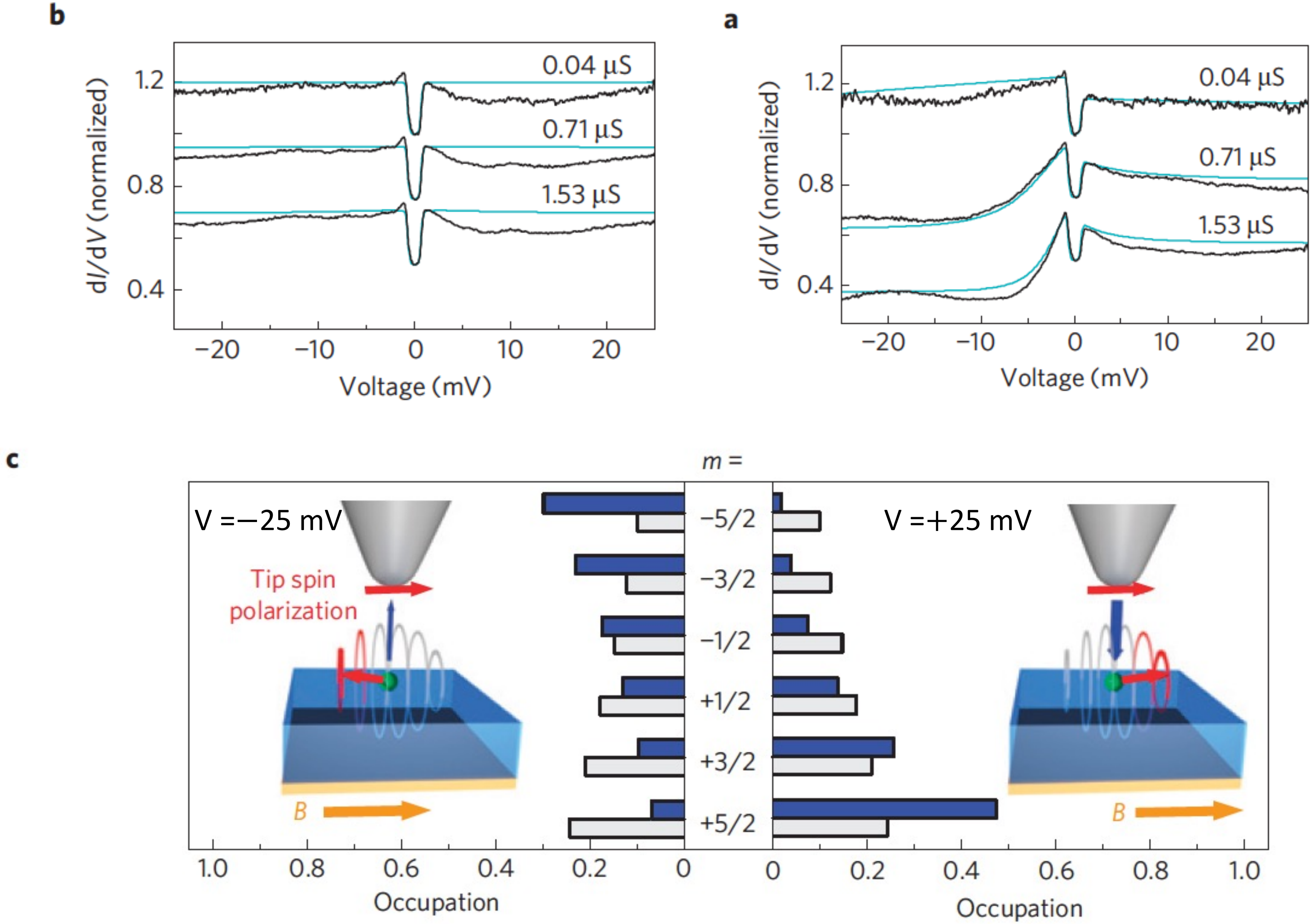


$B = 7$ T
$T = 0.6$ K

Loth et al., Nature Phys. 2010 10.1038/NPHYS1616

Example: Mn/Cu_2N/Cu(100)

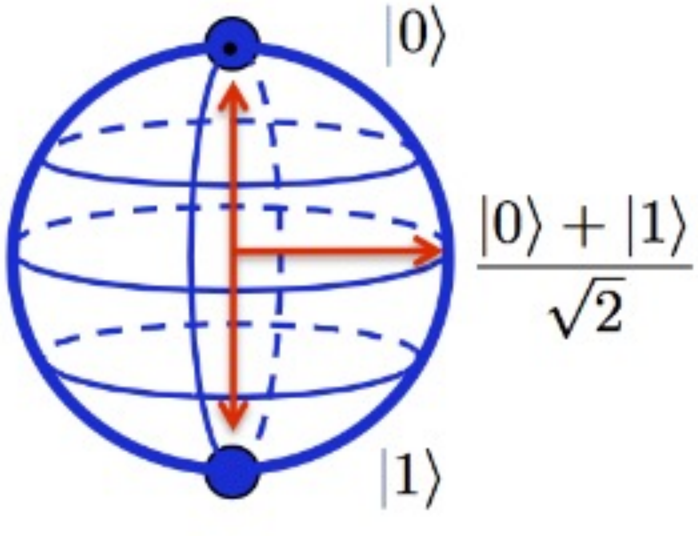
$B = 7$ T
$T = 0.6$ K



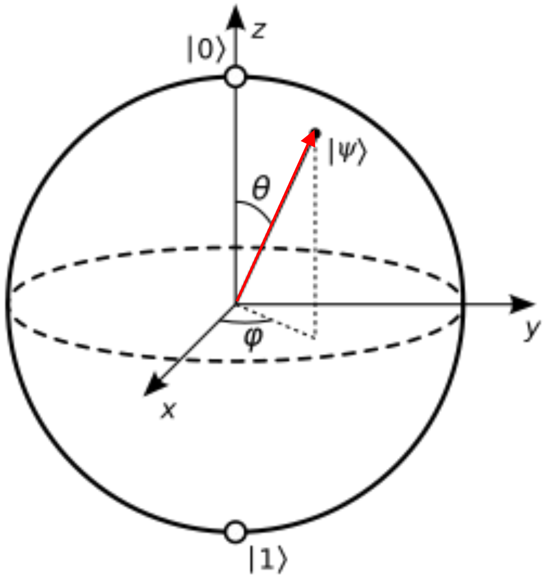
Time-average occupation probabilities of the six Mn spin states for high tunnelling current from the spin-polarized tip (blue) and the spin-averaging tip (grey)

Classical bits vs qubits

classical bit



qubit



Two-level system

Representation using the Bloch sphere

The coherent superposition state
is a linear combination of states $|0\rangle$ and $|1\rangle$

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

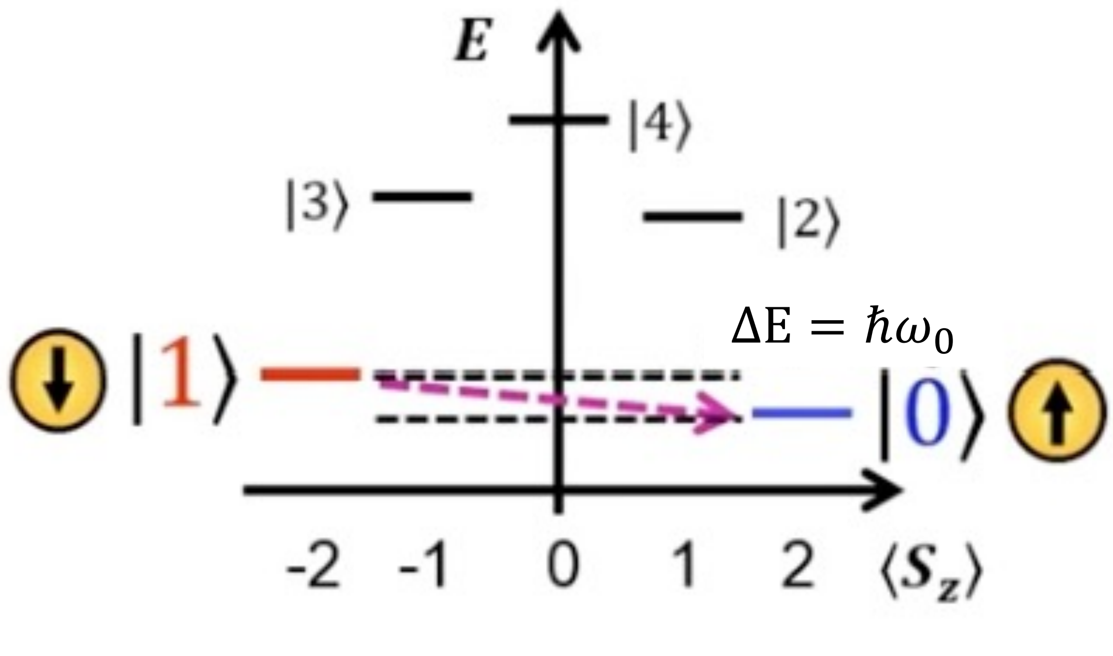
with $|\alpha|^2 + |\beta|^2 = 1$

$$\alpha = \cos\frac{\theta}{2}$$

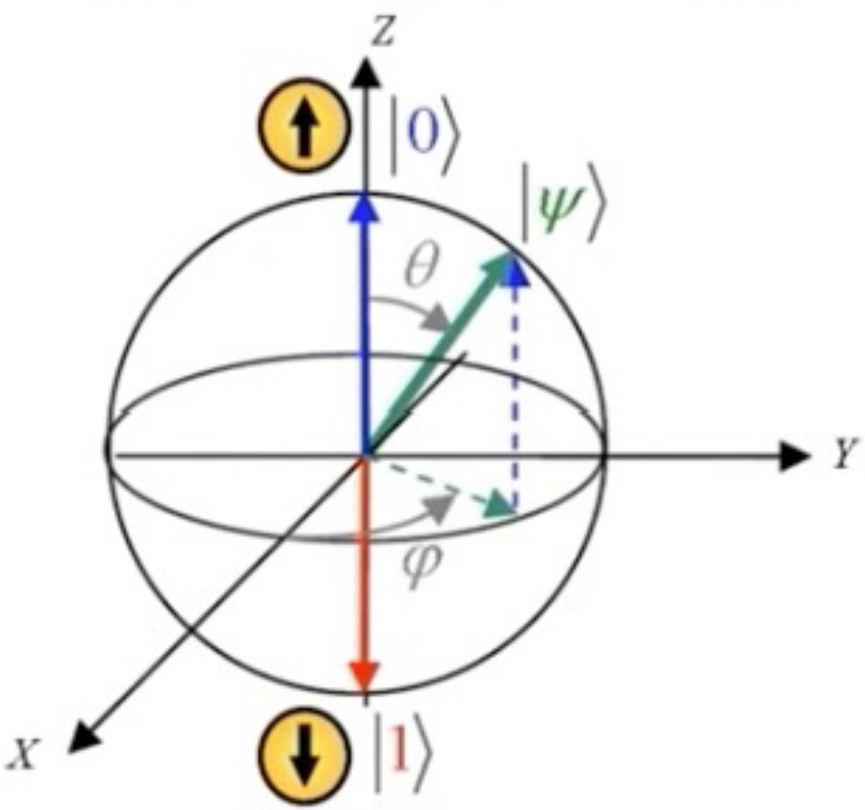
$$\beta = e^{i\varphi}\cos\frac{\theta}{2}$$

https://en.wikipedia.org/wiki/Qubit

Single atoms at surfaces as qubits



$$|\psi\rangle = a|0\rangle + b|1\rangle$$

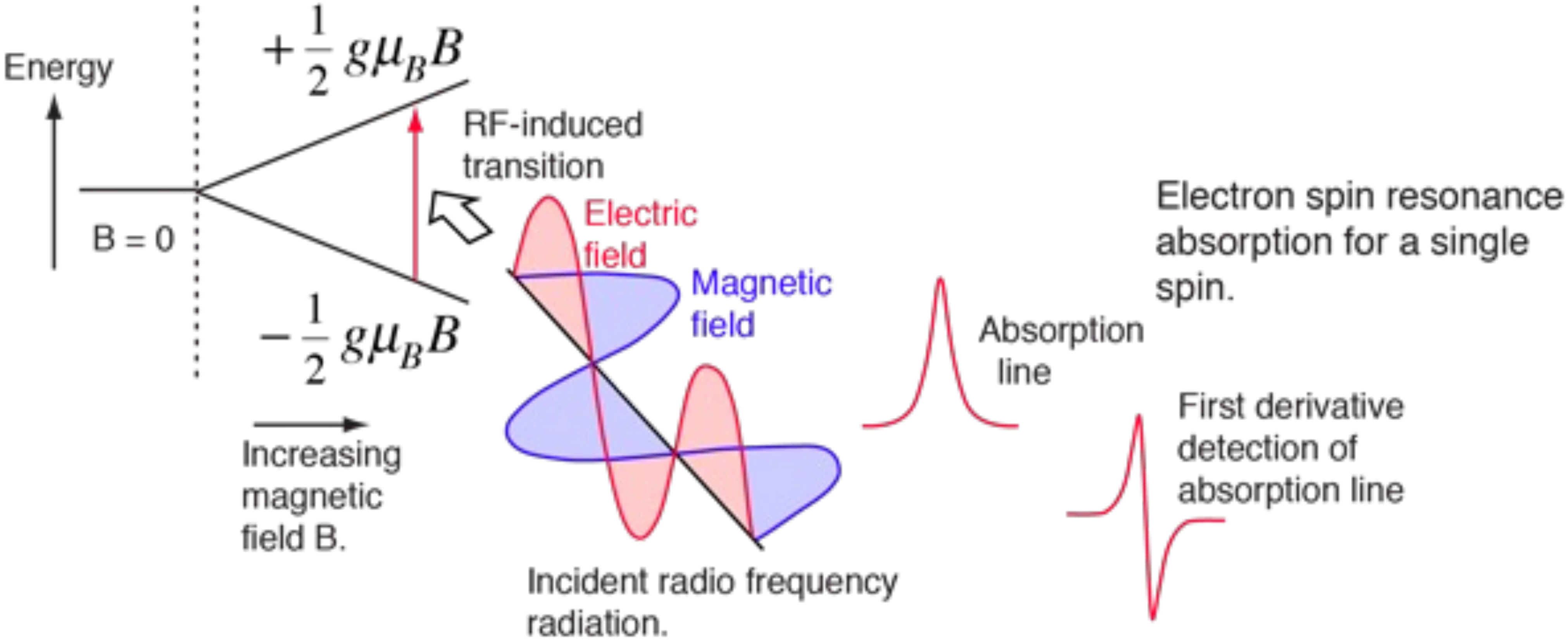


Energy relaxation time T_1
lifetime of state $|1\rangle$

Spin coherence time T_2
lifetime of the superposition state $|\psi\rangle$
(including phase)

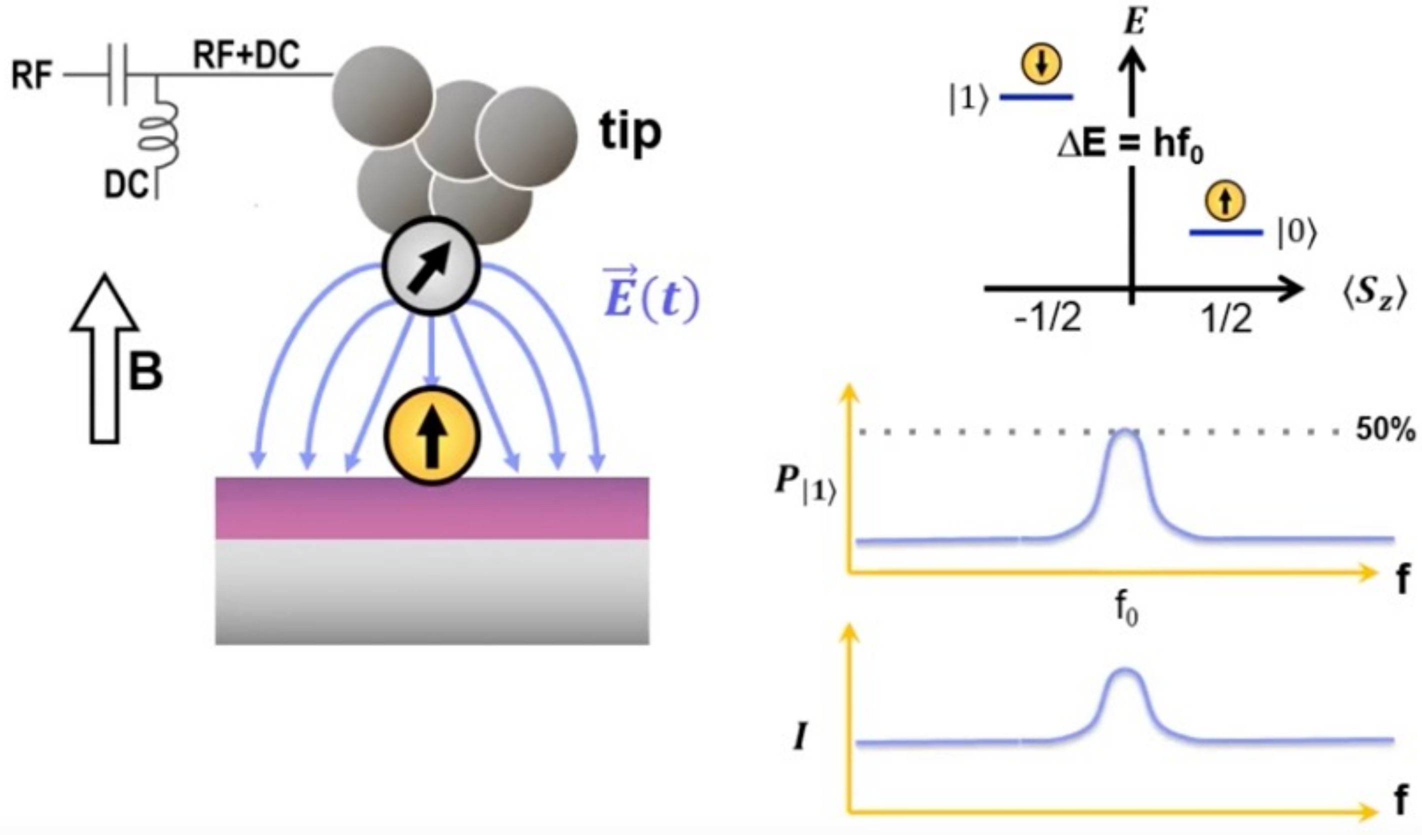
Courtesy of Andreas J. Heinrich, QNS Seoul

Electron Spin Resonance (ESR)



Peak in absorption at the frequency corresponding to the difference in energy

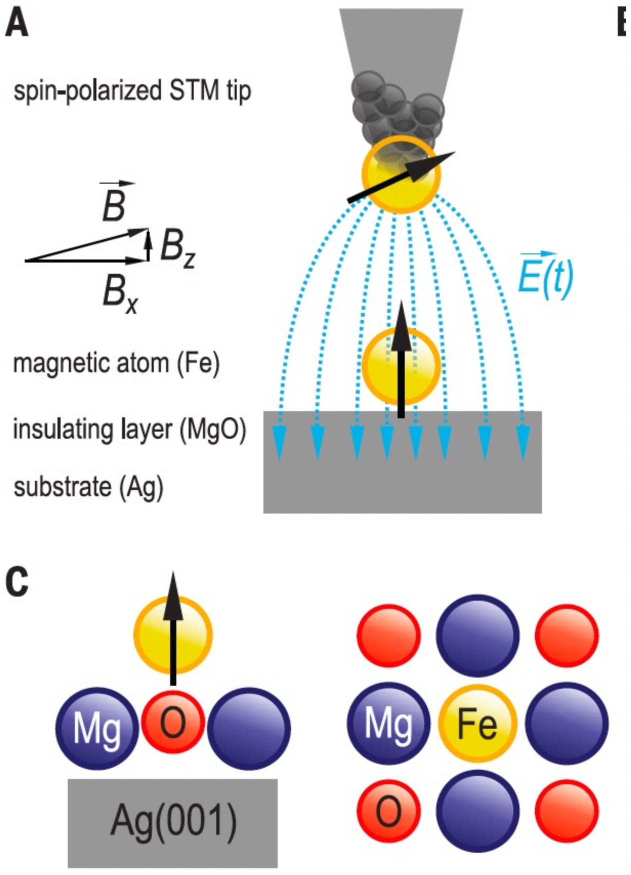
Hyperphysics

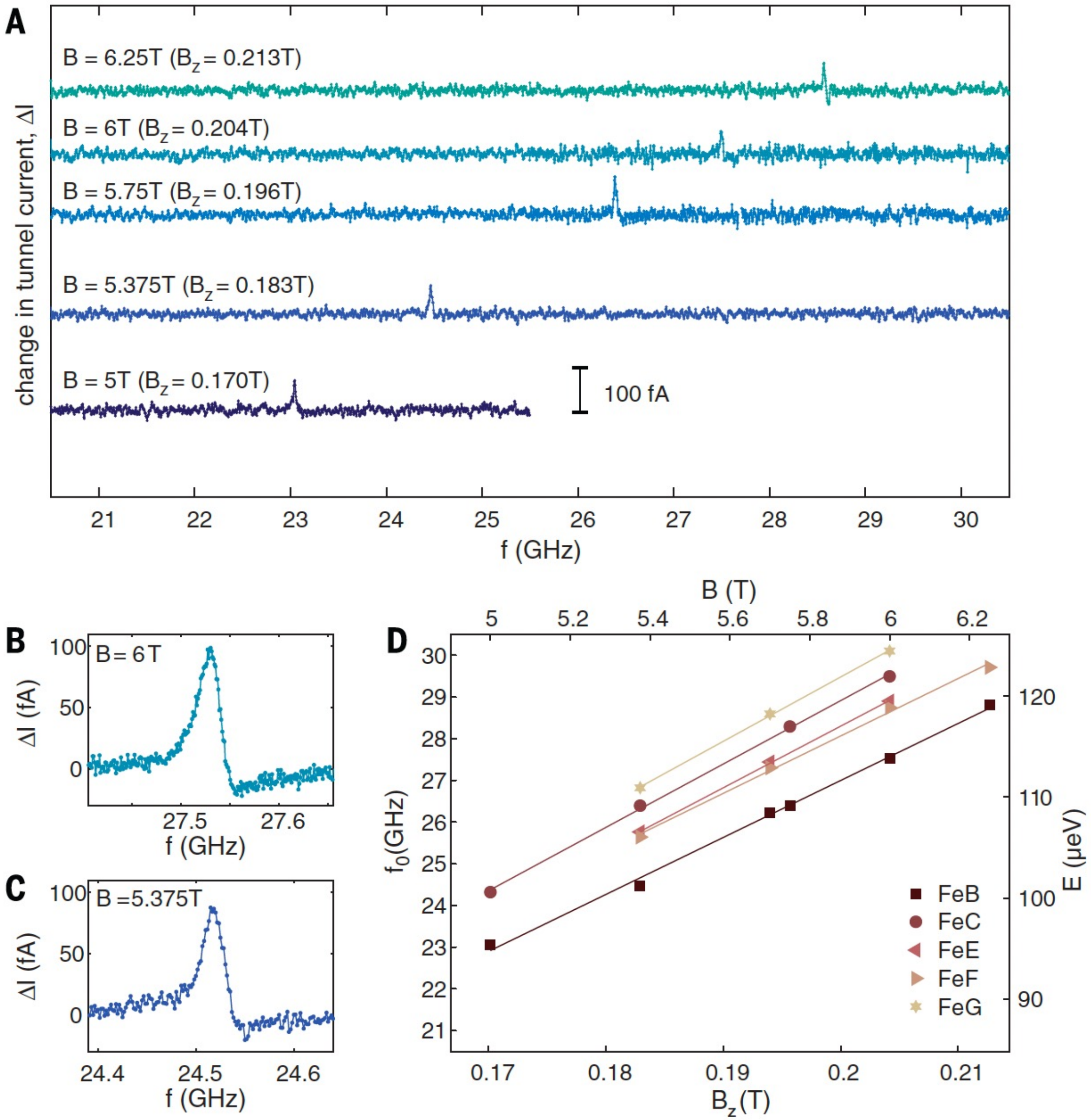


detection by SP-STM

Courtesy of Andreas J. Heinrich, QNS Seoul

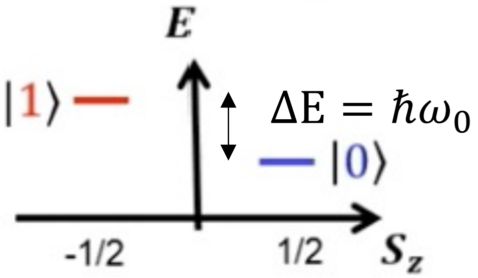
Example: Fe/MgO/Ag(100)



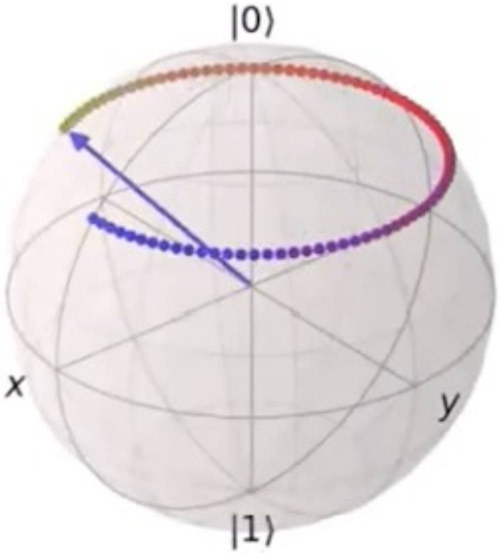


S. Baumann *et al.*, Science **350**, 417 (2015)

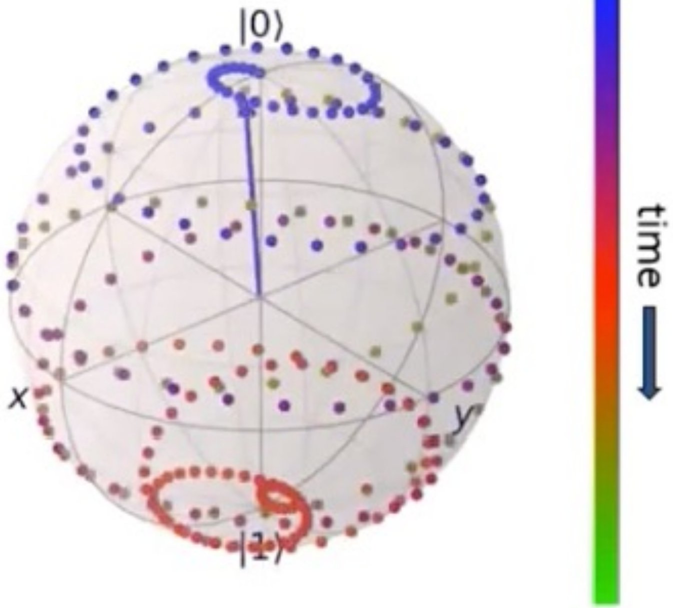
ESR - Rabi oscillations

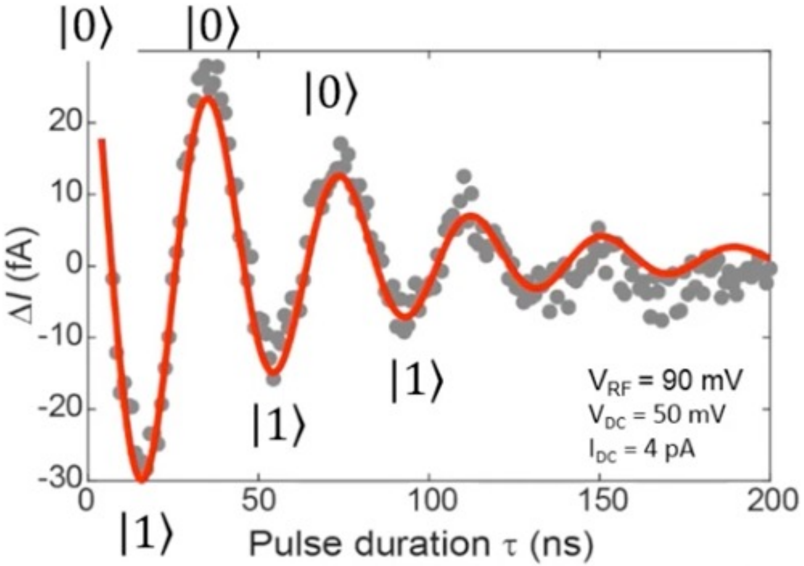


initial state
$|\psi\rangle$



initial state
$|0\rangle$





$H_0 \propto B_0 S_z$ + $H_1 \propto B_1 S_x \cos(\omega_0 t)$

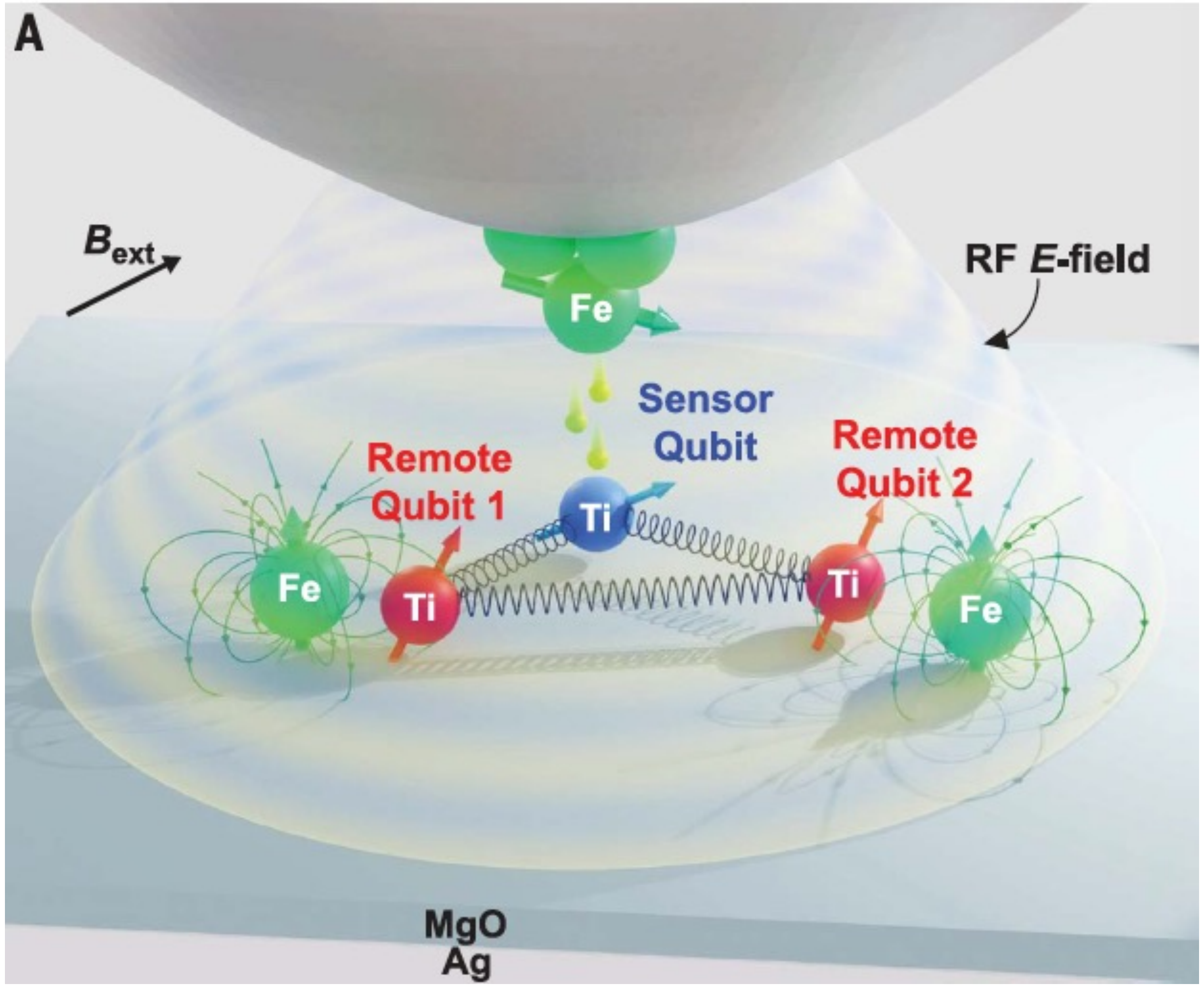
oscillating driving field

→ Rabi oscillation
(z projection of the spin vs time)

decay → coherence time T_2

Courtesy of Andreas J. Heinrich, QNS Seoul

An atomic-scale multi-qubit platform



Wang et al., Science **382**, 87 (2023)