La science quantique

Une vision singulière

XIV) Magnetic Resonance (MR)

et spin qubits

P.A. Besse

Moments magnétiques

et leur Hamiltonien

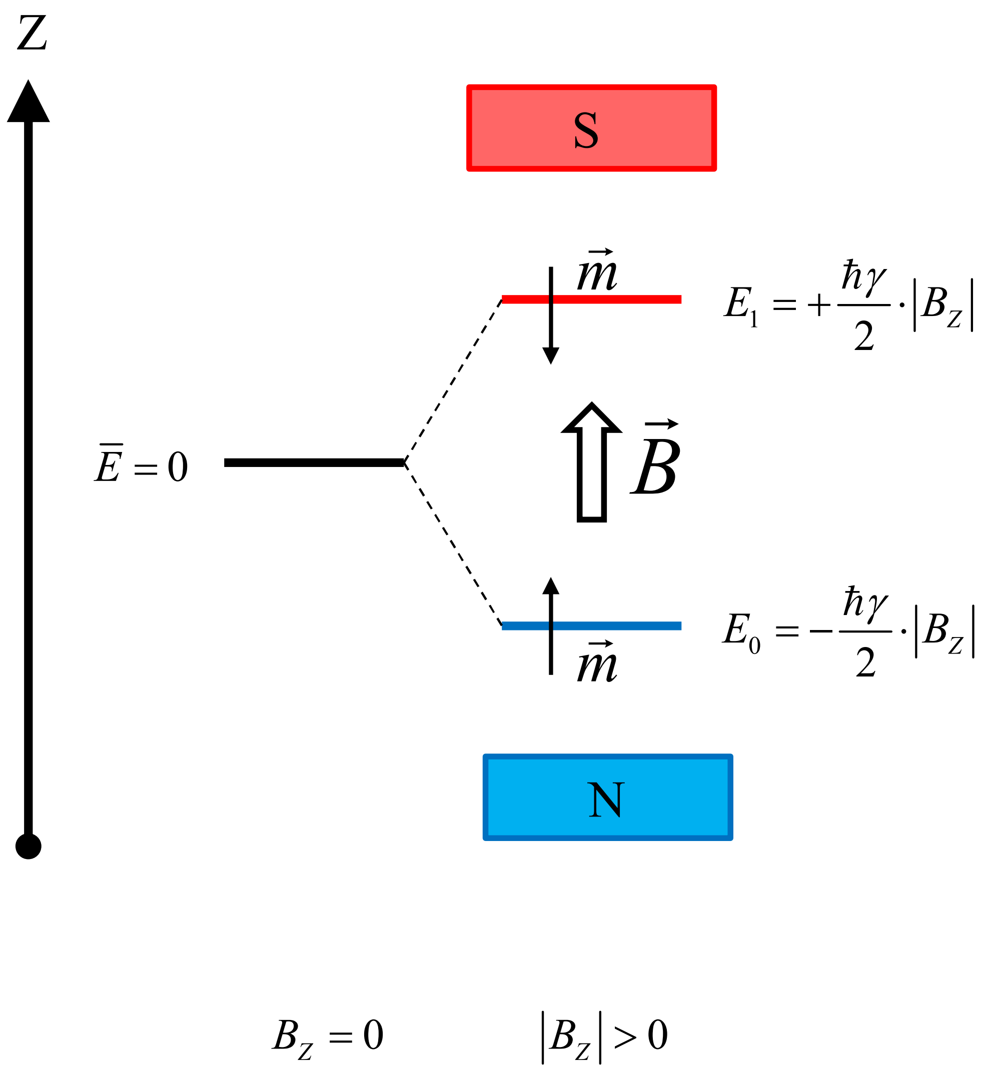
Larmor   Rabi

$$\vec{\vec{H}}_m = -\frac{\hbar\gamma}{2}\cdot\left(B_{Z0}\cdot\vec{\vec{\sigma}}_Z + B_X(\omega)\cdot\vec{\vec{\sigma}}_X\right)$$

DC   AC

$$\gamma \equiv \frac{q}{2m} g_B$$

Moments magnétiques



Etat quantique:

$$|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

a_0 ← «ground state» $|\uparrow\rangle$

a_1 ← «excited state» $|\downarrow\rangle$

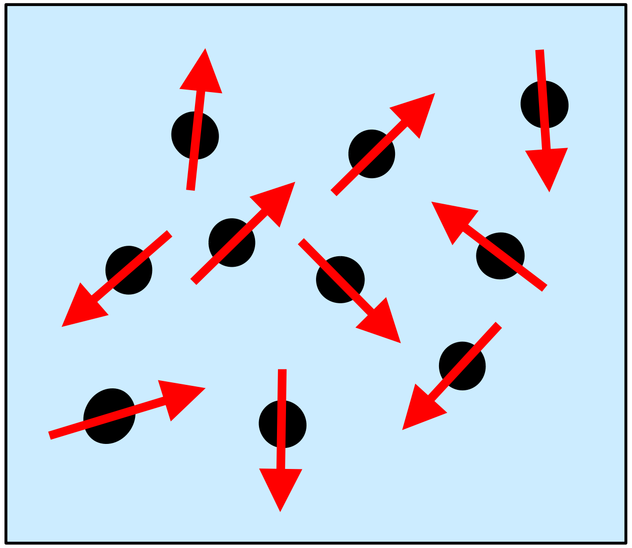
Hamiltonien:

$$\gamma \equiv \frac{q}{2m} g_B$$

$$H = -\vec{m} \cdot \vec{B} = -\frac{\hbar\gamma}{2} |B_Z| \cdot \sigma_Z = \begin{pmatrix} -\frac{\hbar\gamma}{2}|B_Z| & 0 \\ 0 & +\frac{\hbar\gamma}{2}|B_Z| \end{pmatrix}$$

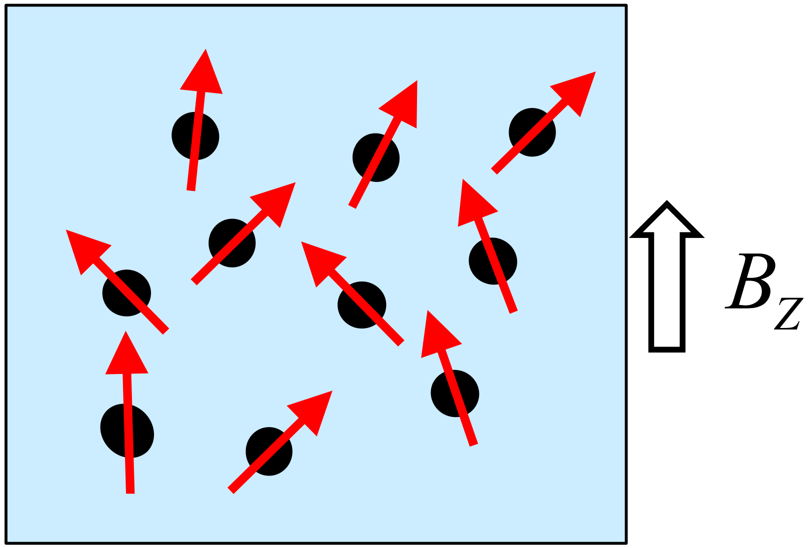
Magnétisation moyenne

Sans champ magnétique



$$\left\langle \vec{M} \right\rangle = 0$$

Avec un champ Bz



$$\left\langle \vec{M} \right\rangle = N \cdot \frac{\hbar\gamma}{2} \cdot \frac{e^{-E_0/kT} - e^{-E_1/kT}}{e^{-E_0/kT} + e^{-E_1/kT}} \cdot \vec{n}_z$$

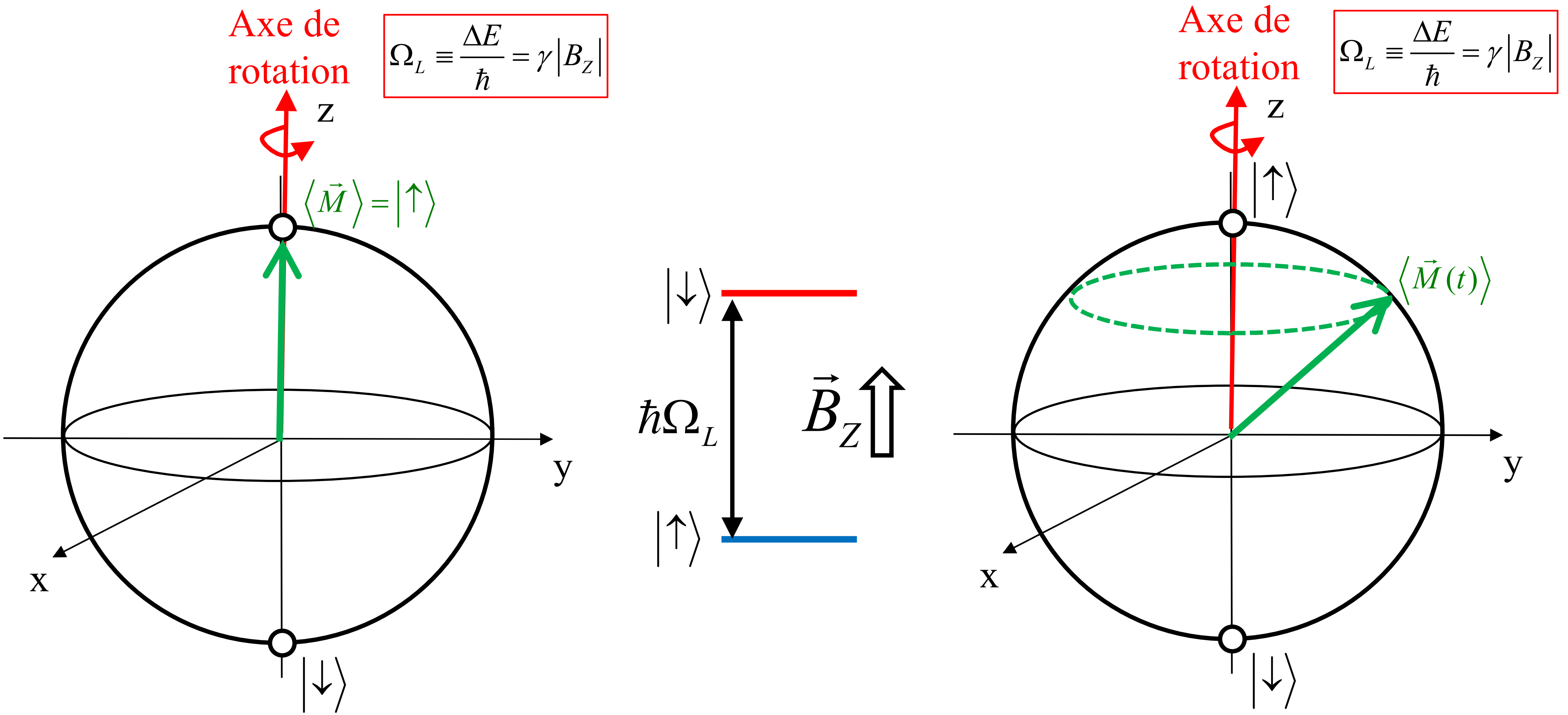
$$\left\langle \vec{M} \right\rangle = N \cdot \frac{\hbar\gamma}{2} \cdot th\left(\frac{\Delta E}{2kT}\right) \cdot \vec{n}_z$$

$$\Delta E \equiv \hbar\gamma \cdot \left|B_Z\right|$$

$$\gamma \equiv \frac{q}{2m} g_B$$

Larmor et relaxation

A l'équilibre **En état superposé**

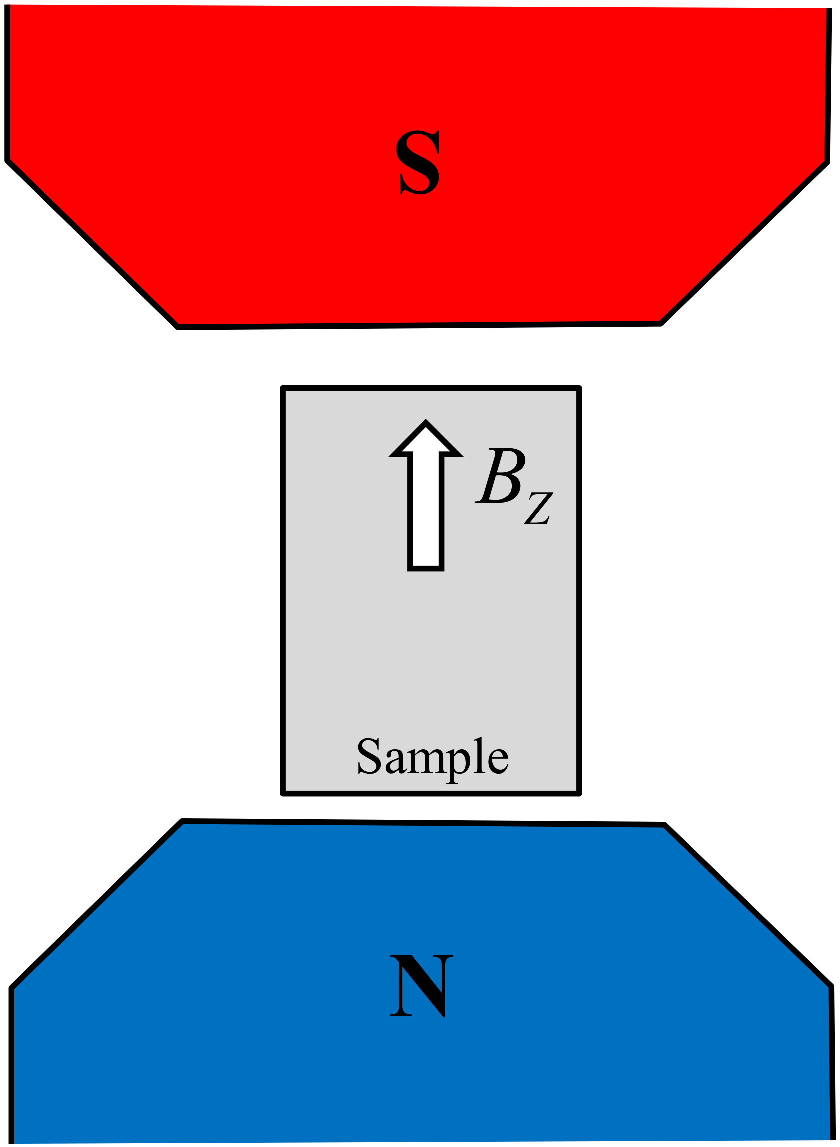


Nuclear Magnetic Resonance (NMR):

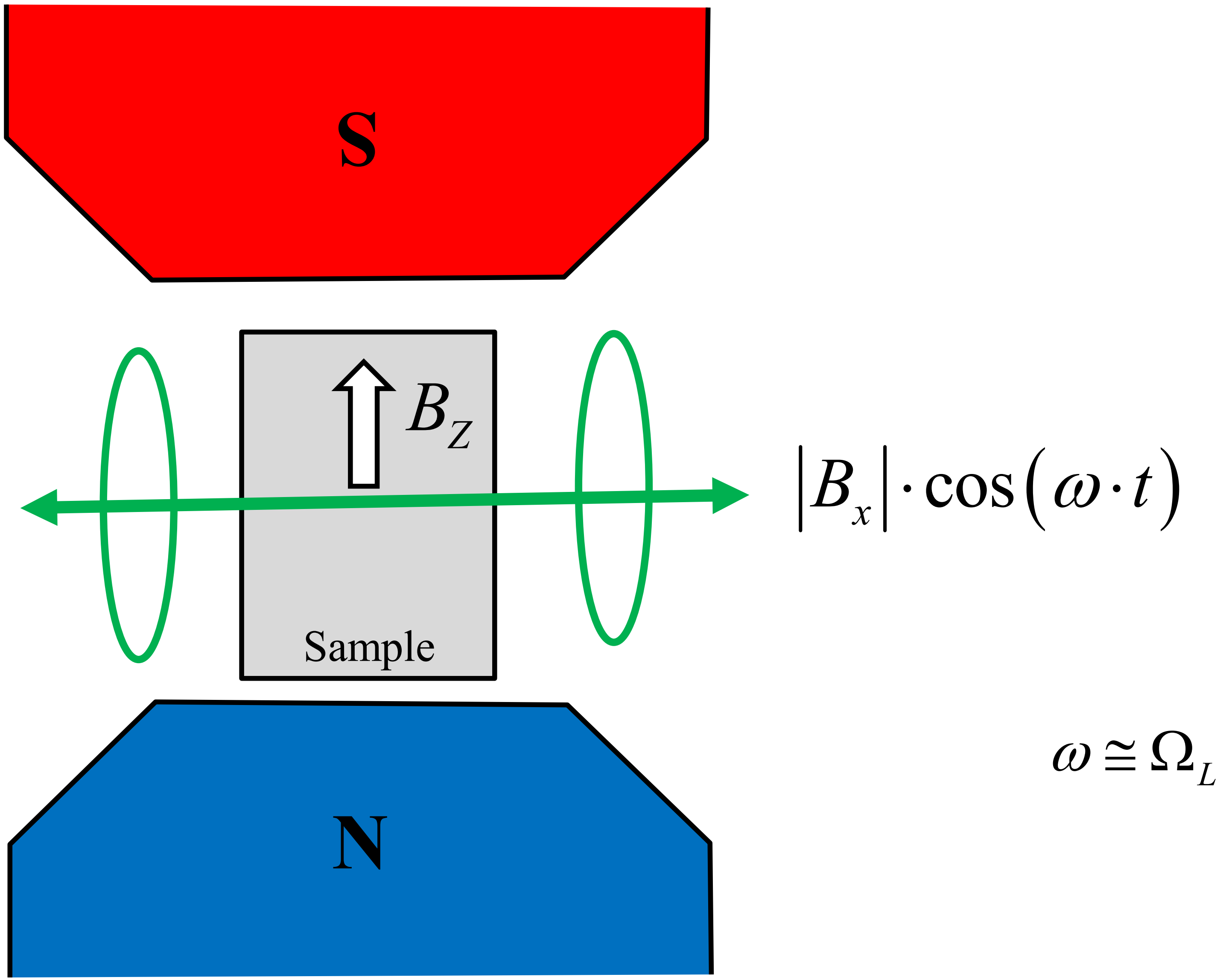
Mesure des spins des noyaux

(en particulier du proton = Hydrogène)

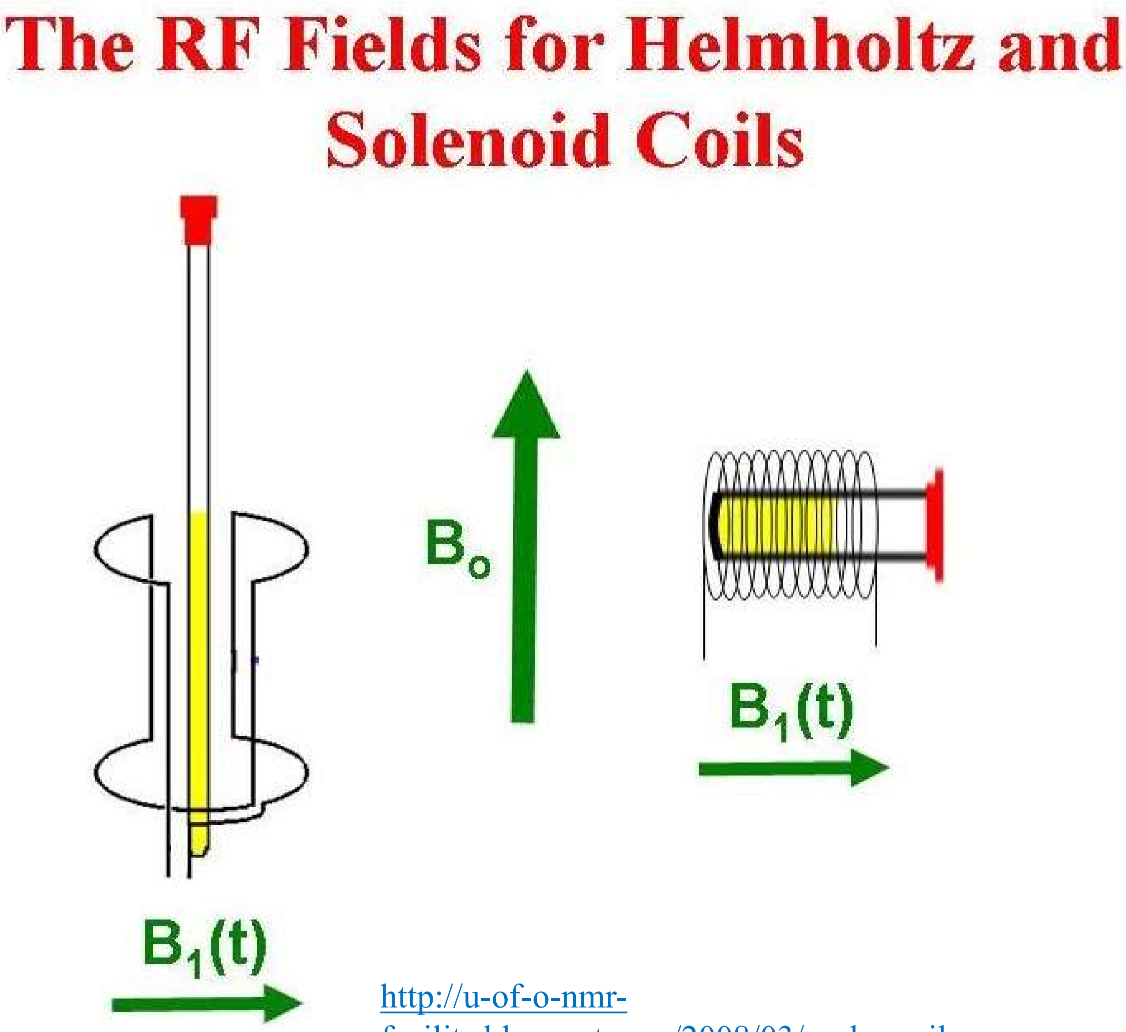
1) Polarisation par un fort champ magnétique DC en Z



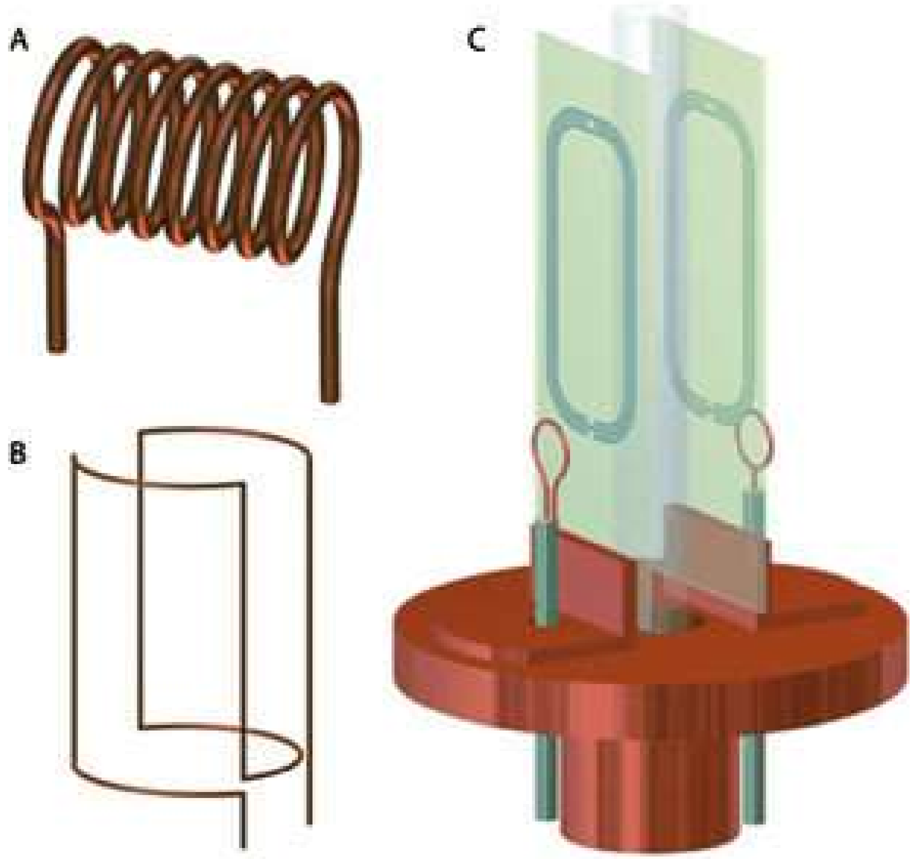
2) Excitation RF selon l'axe X



Variantes de bobines d’excitation et de détection RF

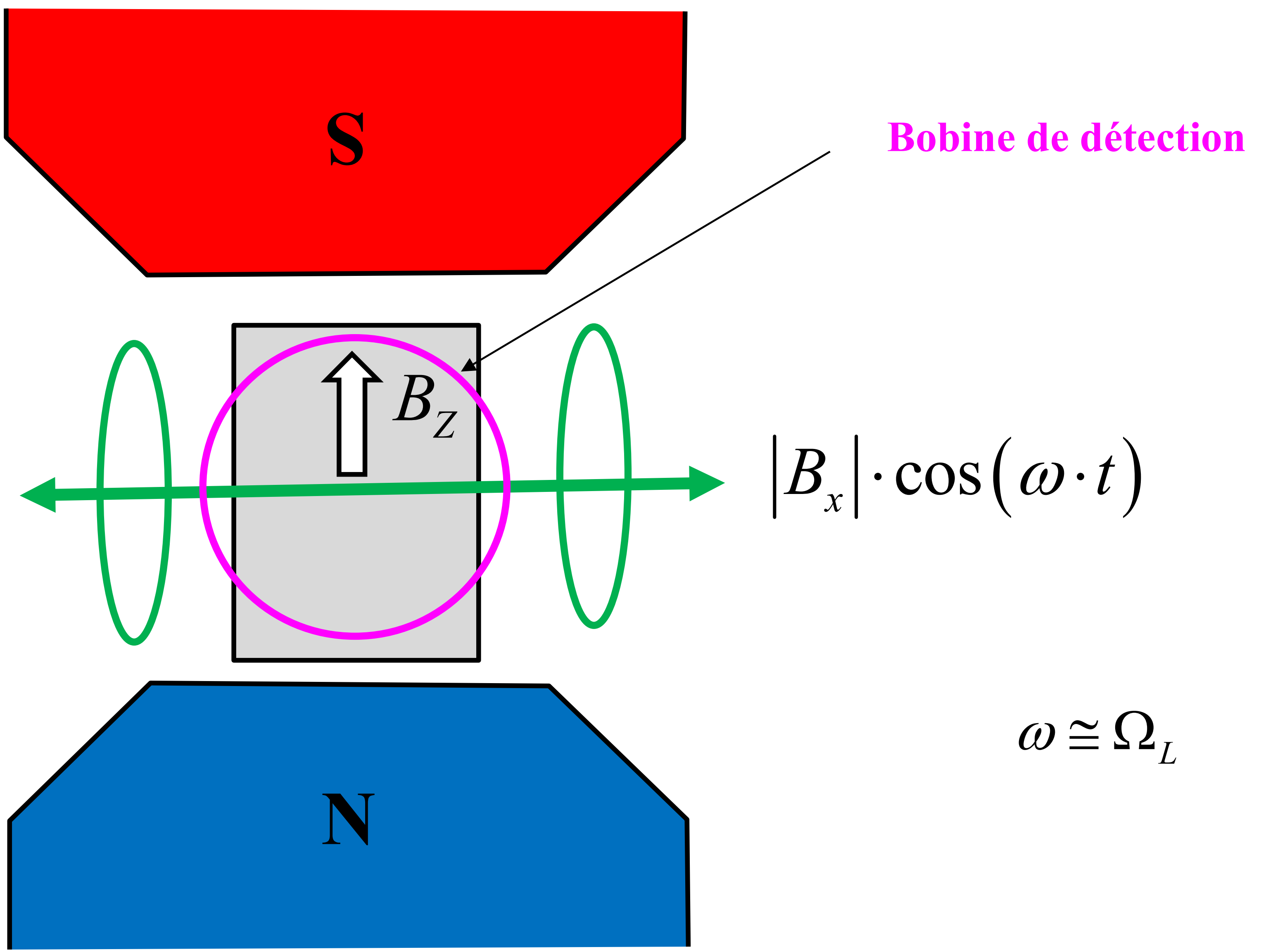


http://u-of-o-nmr-facility.blogspot.com/2008/03/probe-coil-geometry.html?m=1

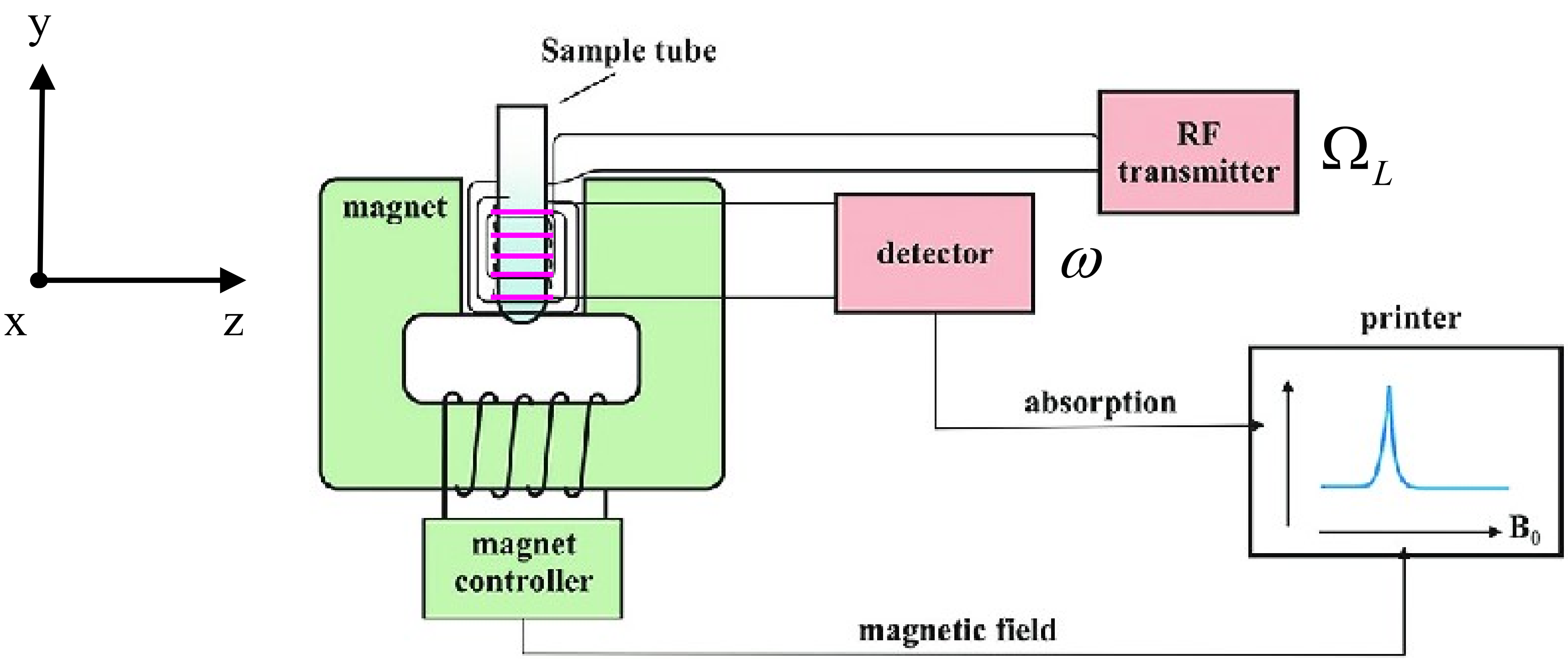


https://www.researchgate.net/figure/Common-NMR-coil-geometries-A-solenoid-B-saddle-coil-C-inductively-coupled-HTS-coils_fig16_279729103

3) Détection RF selon l'axe Y

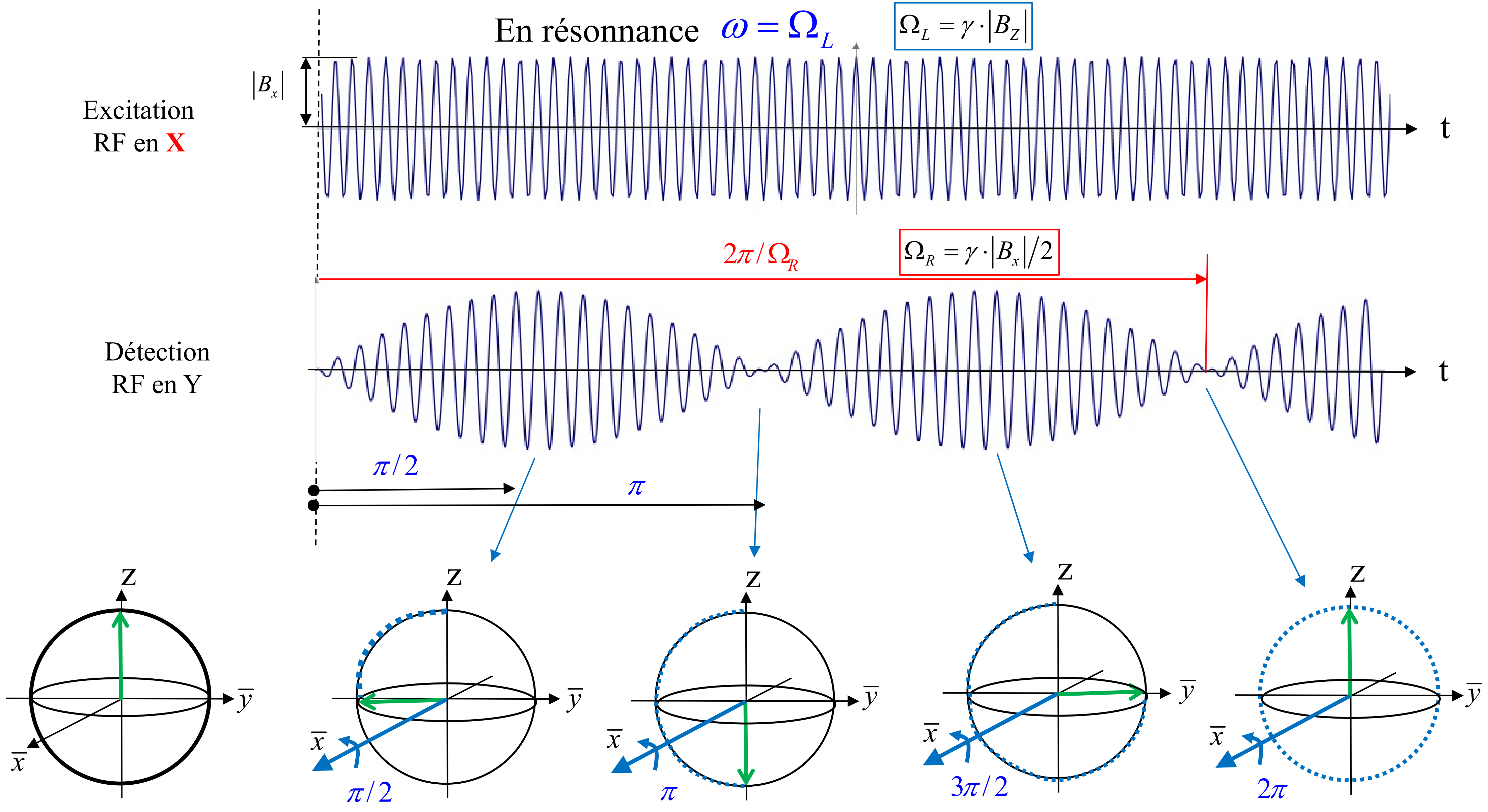


The MR Spectrometer

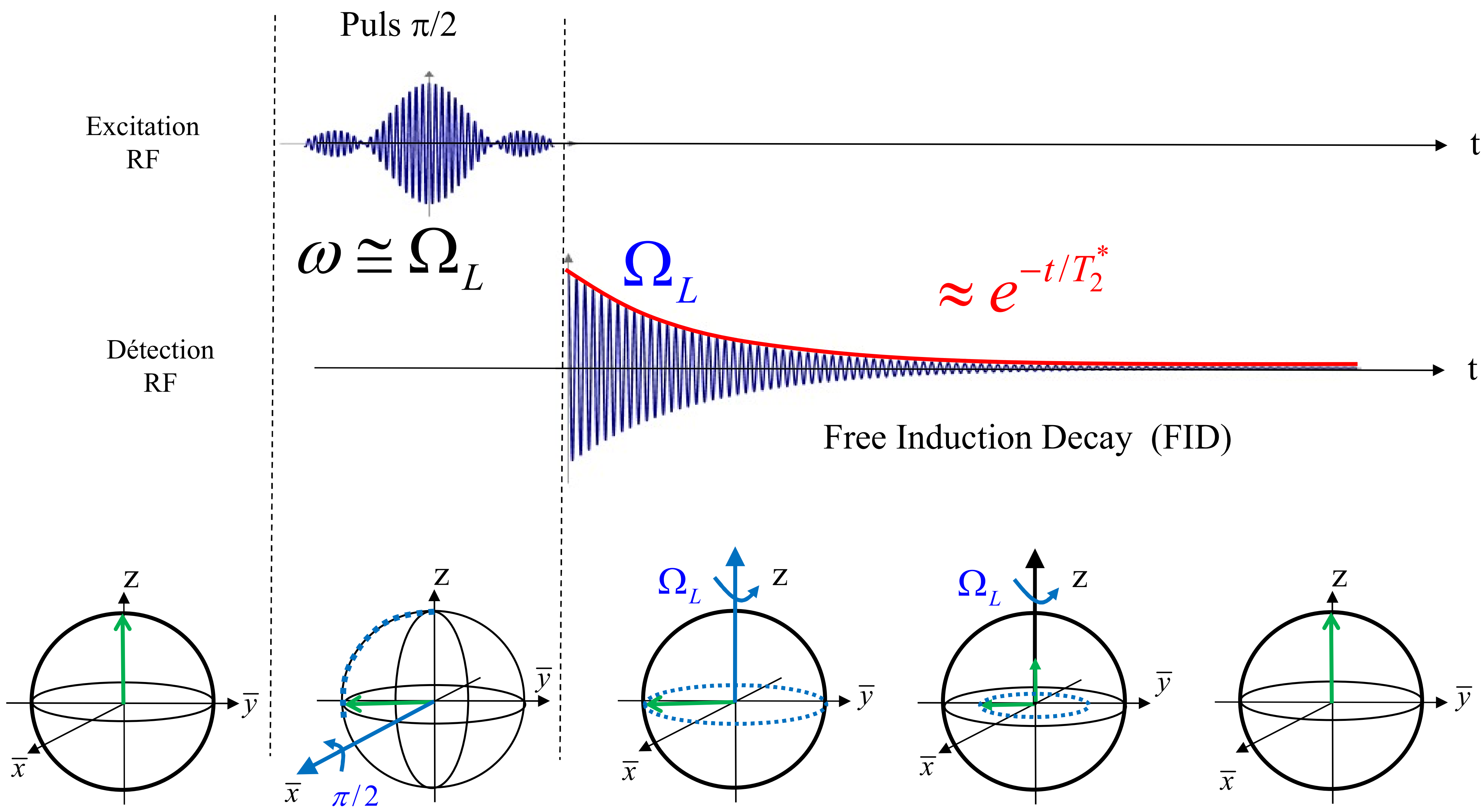


https://www.youtube.com/watch?v=3gy9Mab2RZg

Oscillations de Rabi (1)

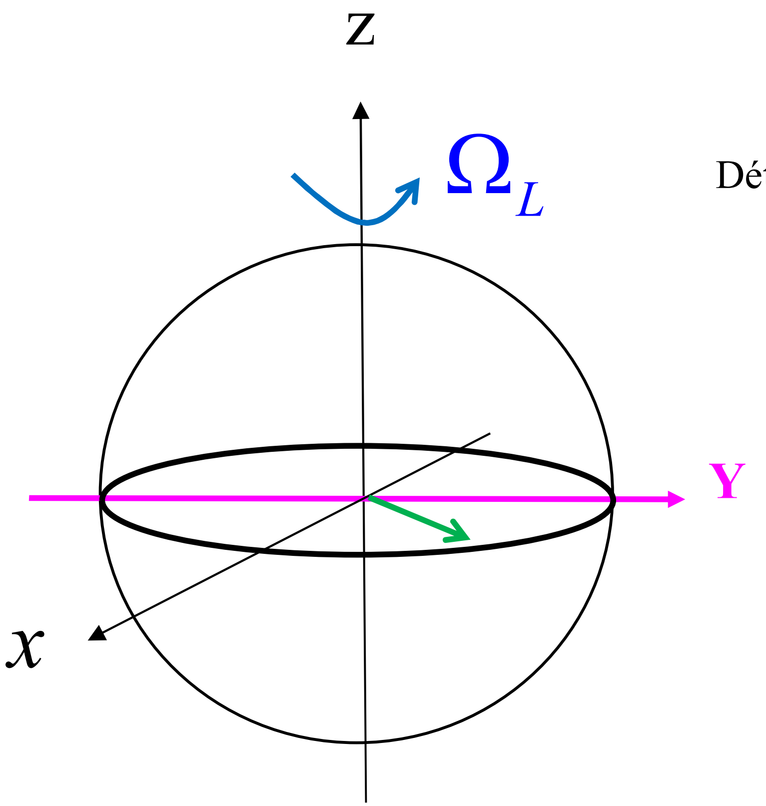


Relaxation et Free Induction Decay (FID)

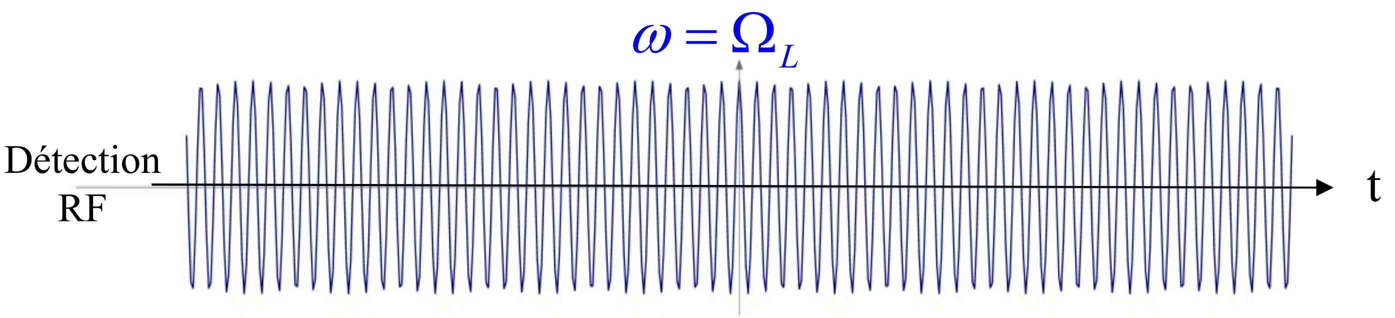


PAB

Principe de détection:
Mesure en Y dans le référentiel fixe

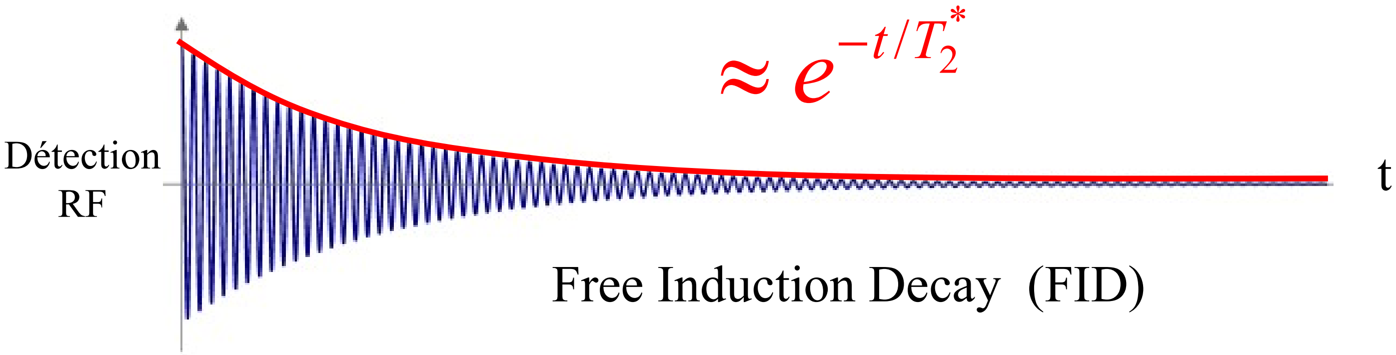


Sans relaxation **(signal détecté en Y):**



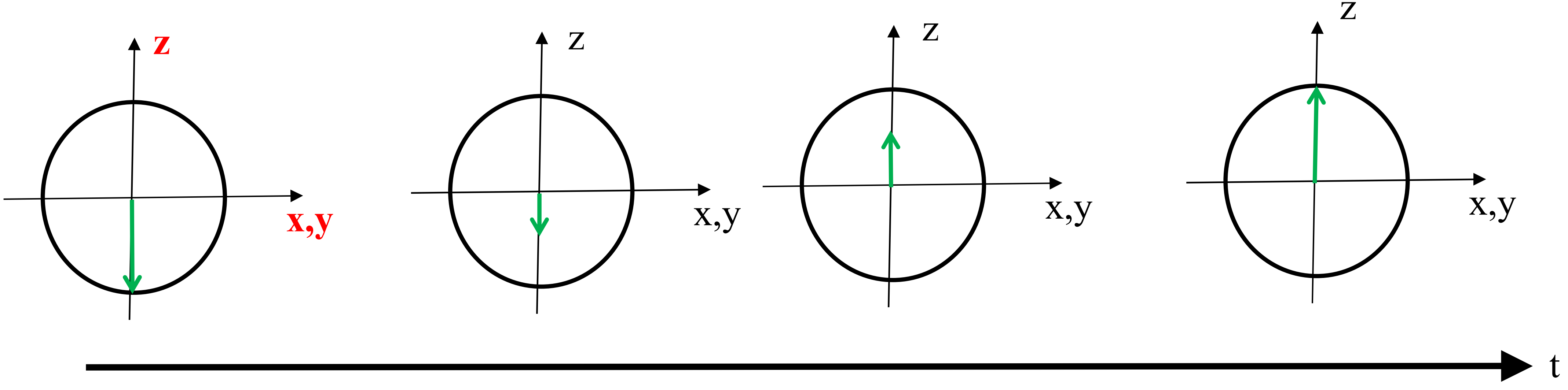
Avec relaxation: Free Induction Decay (FID)

Tous les atomes n'ont pas exactement la même fréquence de Larmor
→ Décohérence

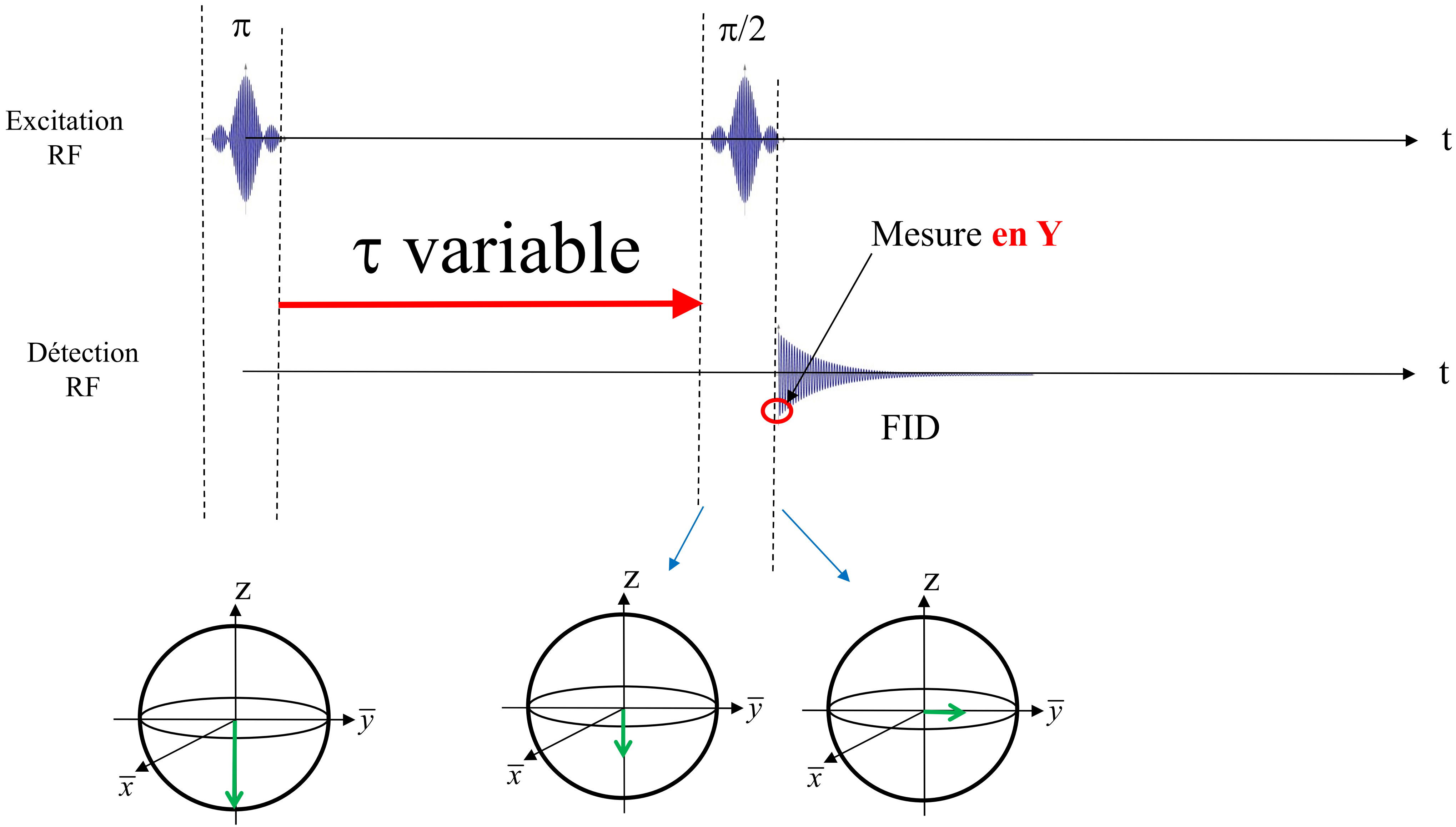


Relaxation

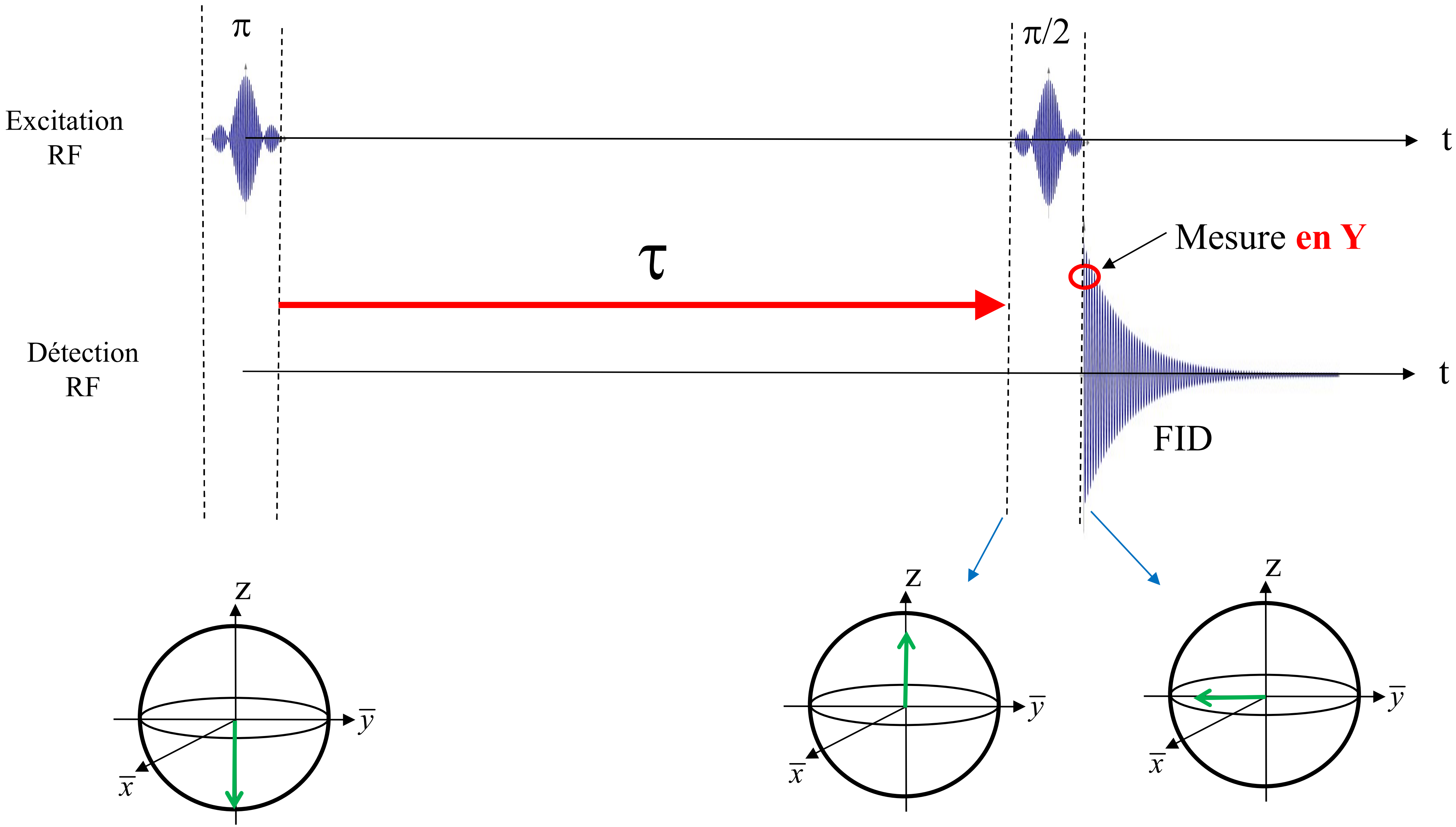
Temps T1



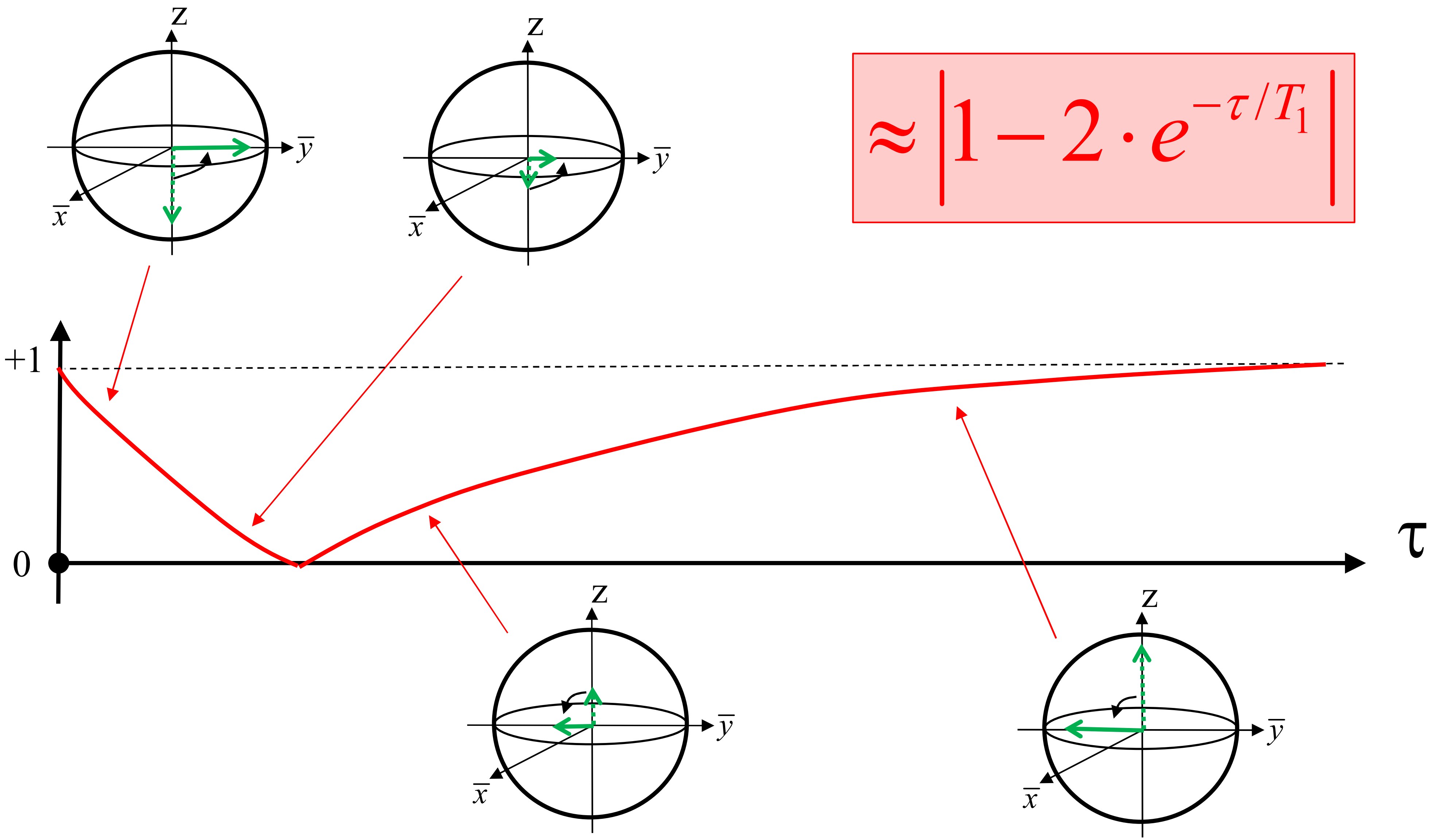
Mesure du temps de relaxation T1



Mesure du temps de relaxation T1



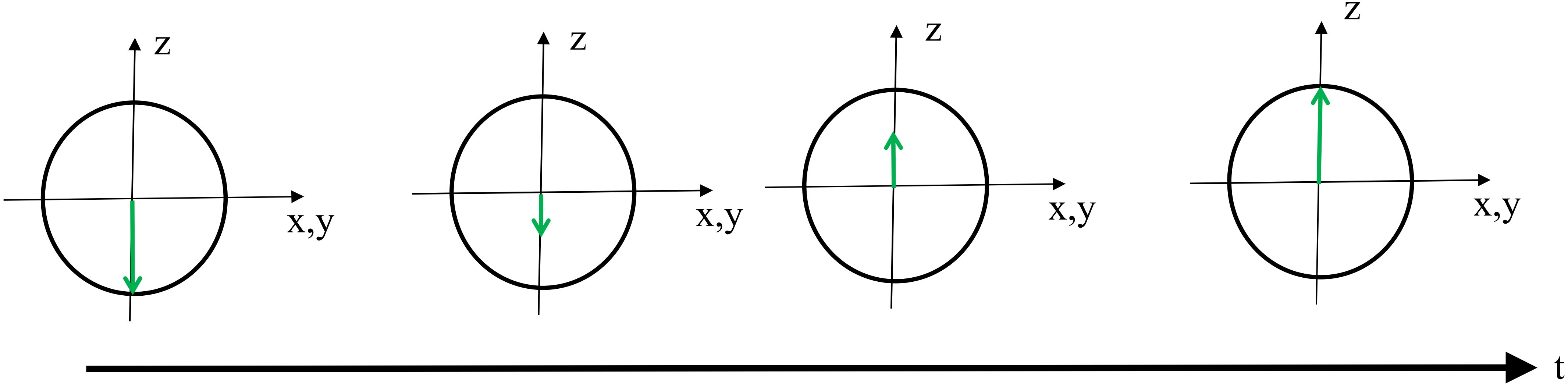
Mesure du temps de relaxation T1



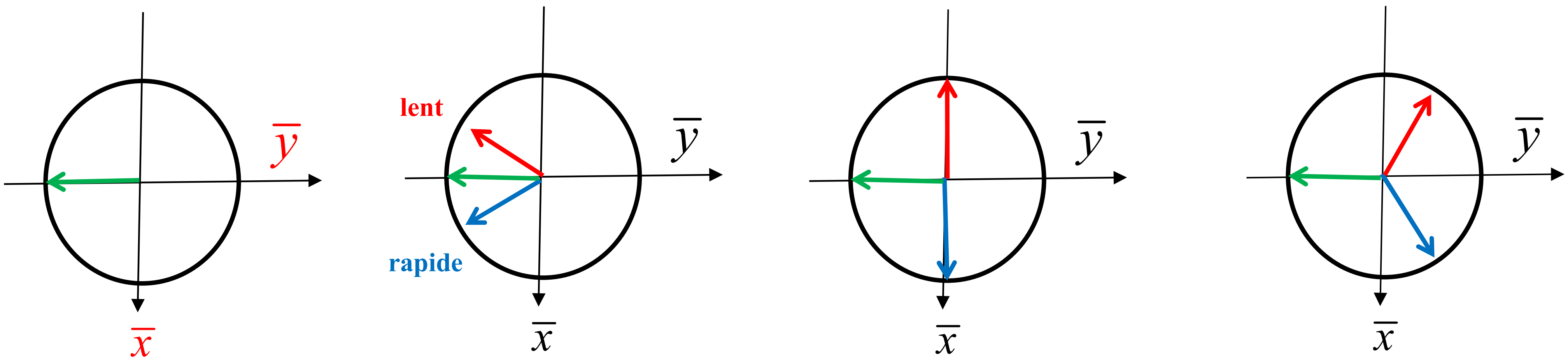
$$\approx \left| 1 - 2 \cdot e^{-\tau / T_1} \right|$$

Relaxation et **décohérence**

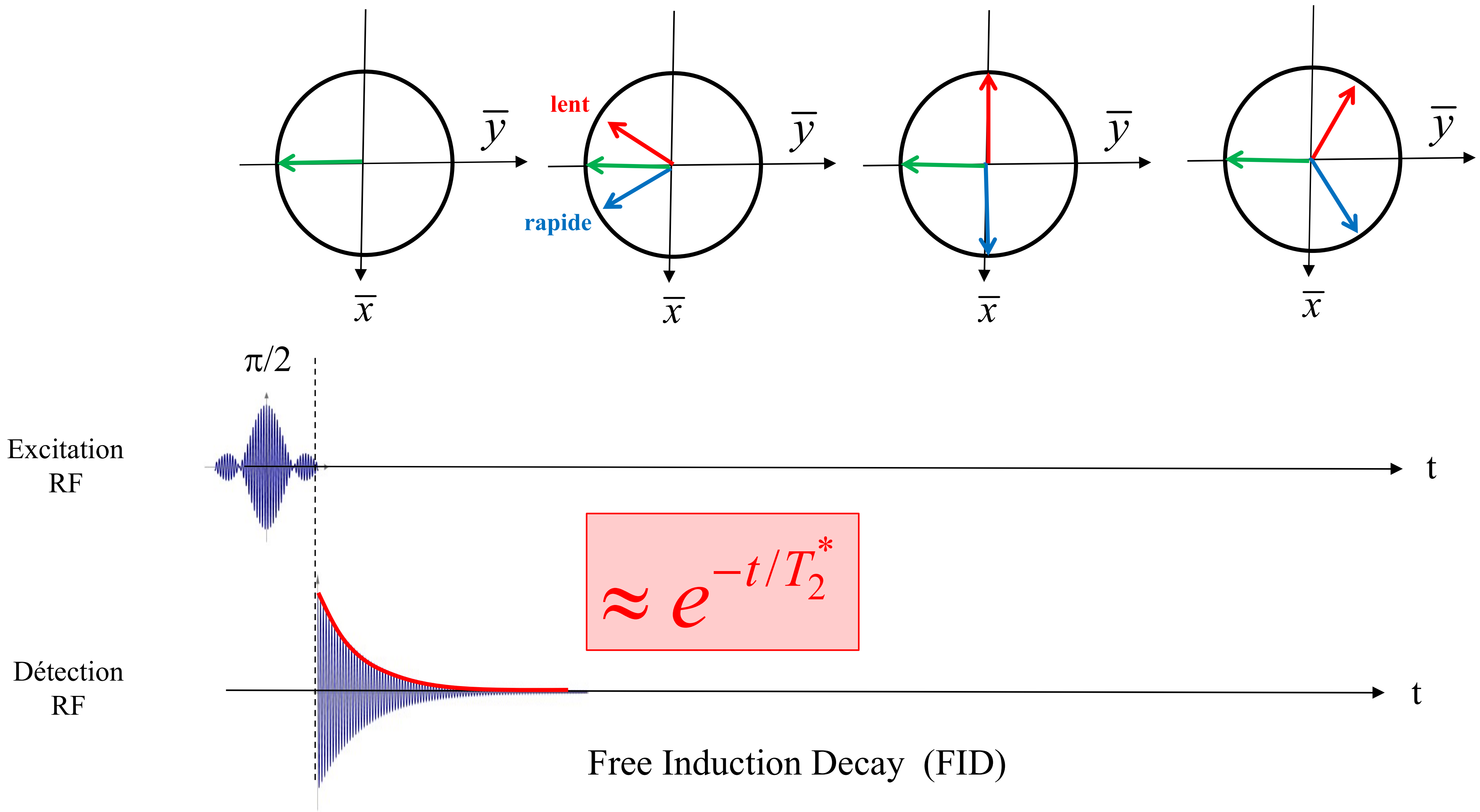
Temps T1



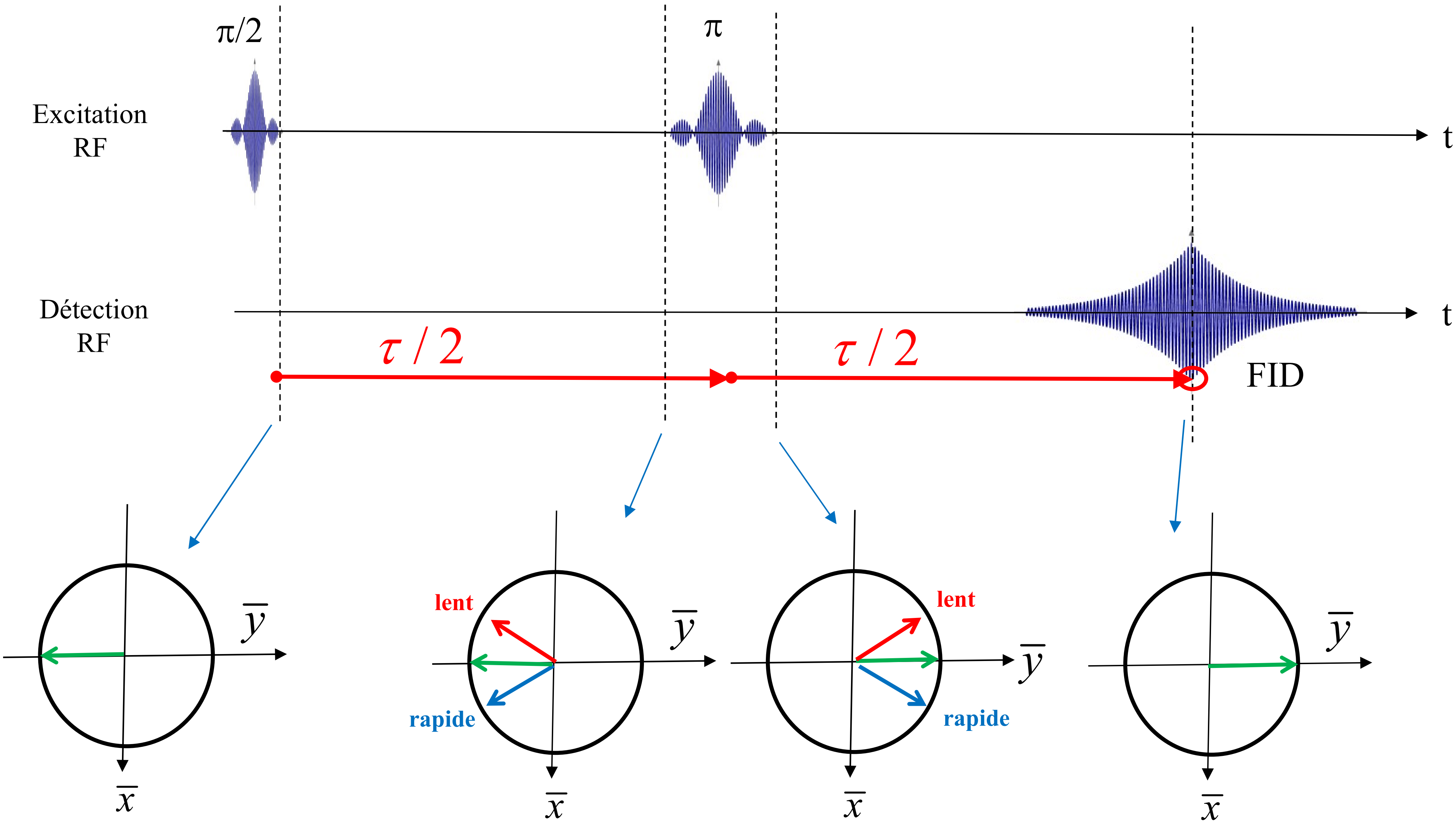
Temps T2* (T2)



Décohérence et temps T2*

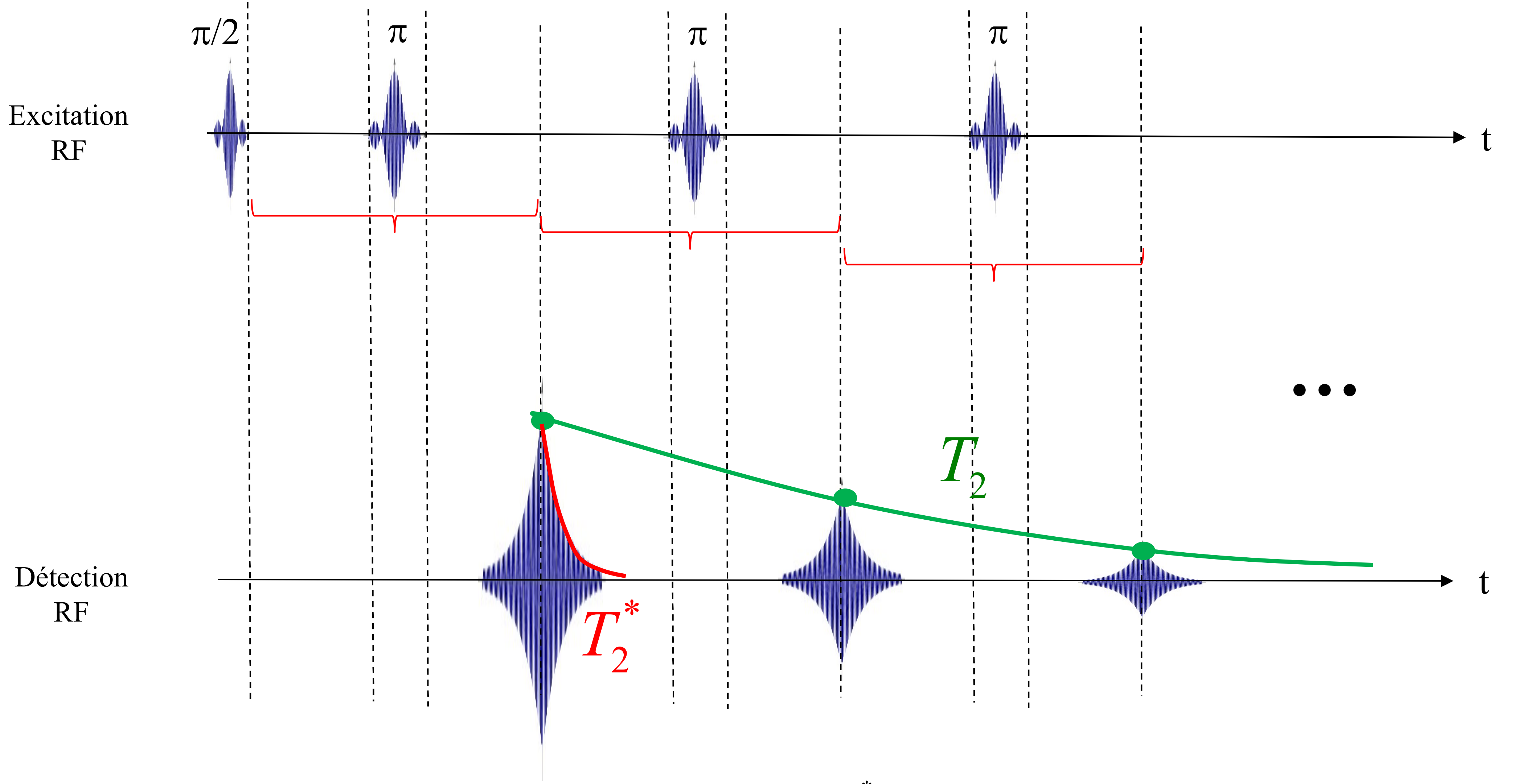


Spin Echo



π/2
π
Excitation RF
t
Détection RF
t
$\tau/2$
$\tau/2$
FID
$\bar{y}$
$\bar{x}$
lent
rapide
lent
rapide

Mesure de T2 et T2*

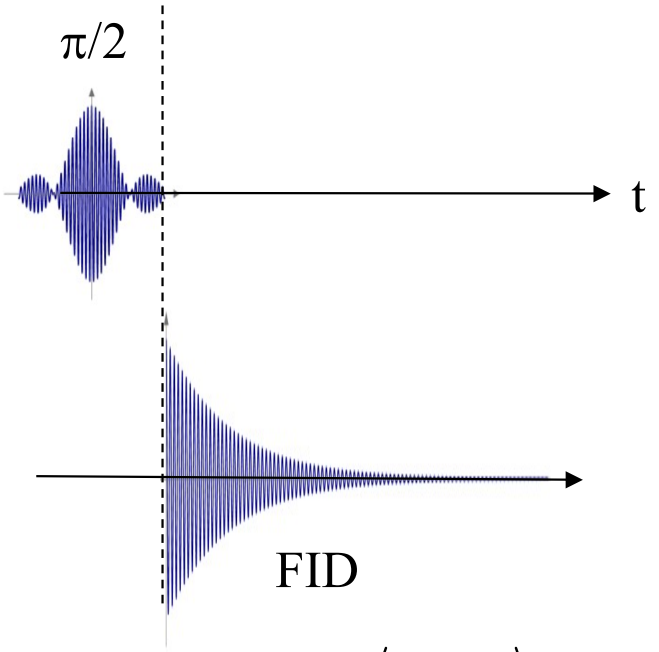


En général: $T_2^* \ll T_2 \ll T_1$

Applications en chimie:

Spectroscopie moléculaire

1D spectroscopie



$\langle M_y(t) \rangle$

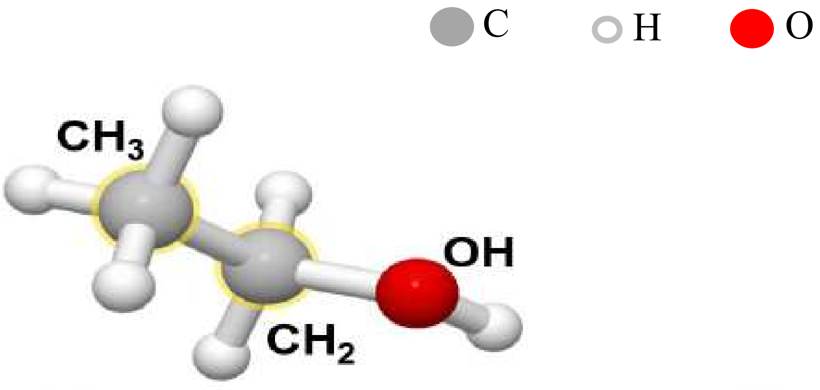
Fourier ⇩

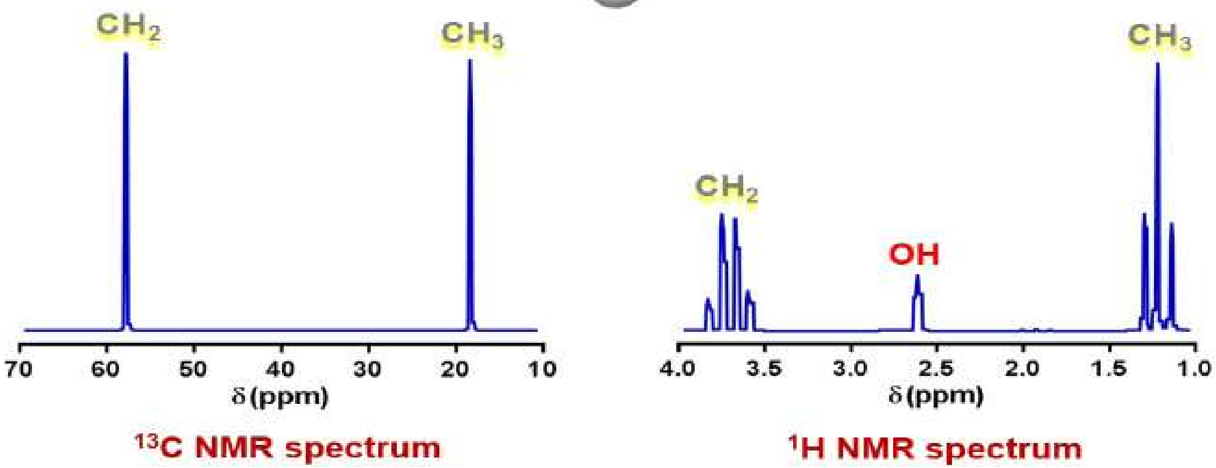
$\langle \tilde{M}_y(f) \rangle$

- Fréquences
- Intensités
- Largueurs de ligne

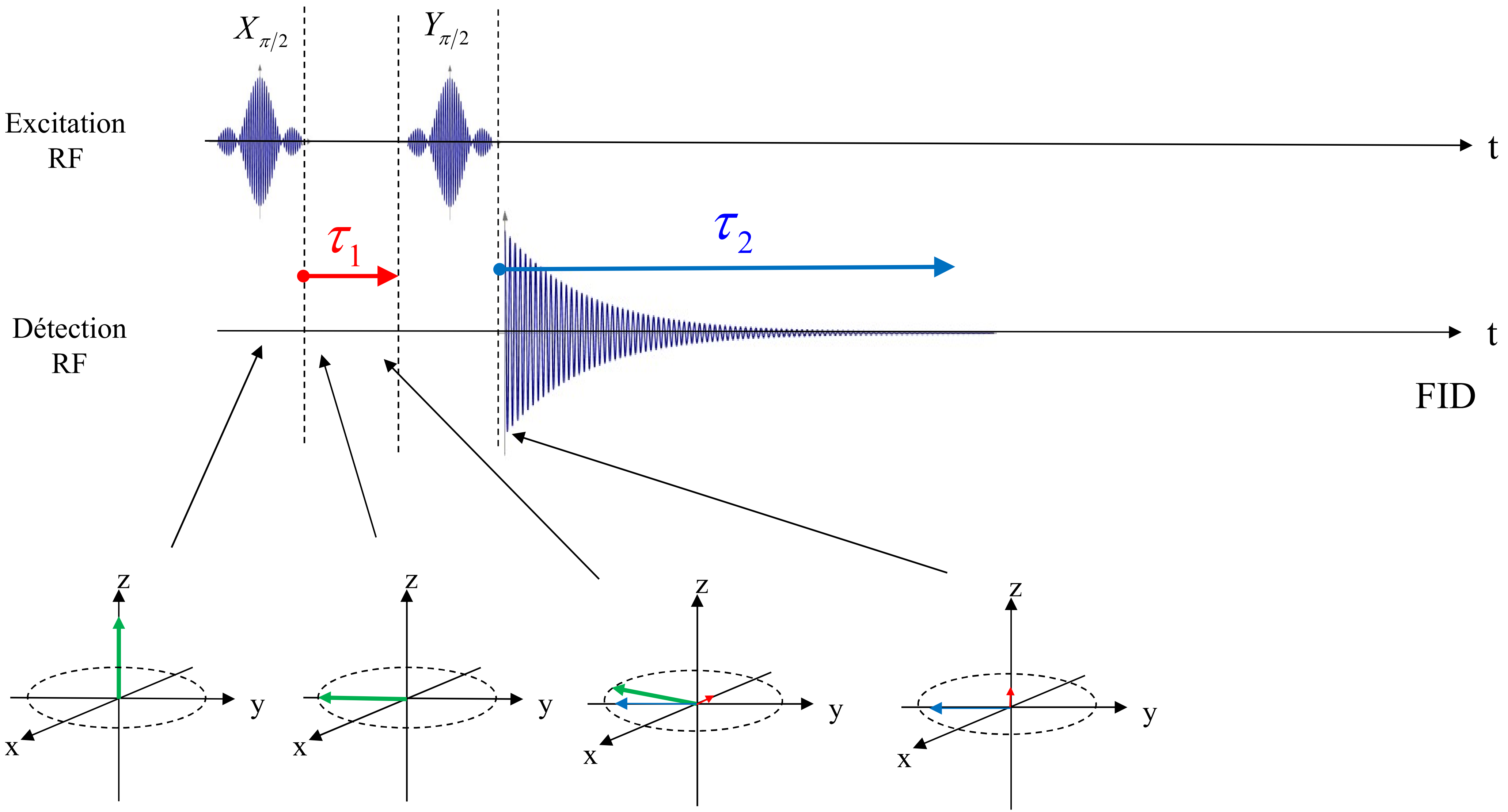
https://www.researchgate.net/figure/Typical-NMR-spectra-for-ethanol-molecule-On-the-left-the-13-C-NMR_fig3_273219251

Exemple: éthanol C_2H_5OH

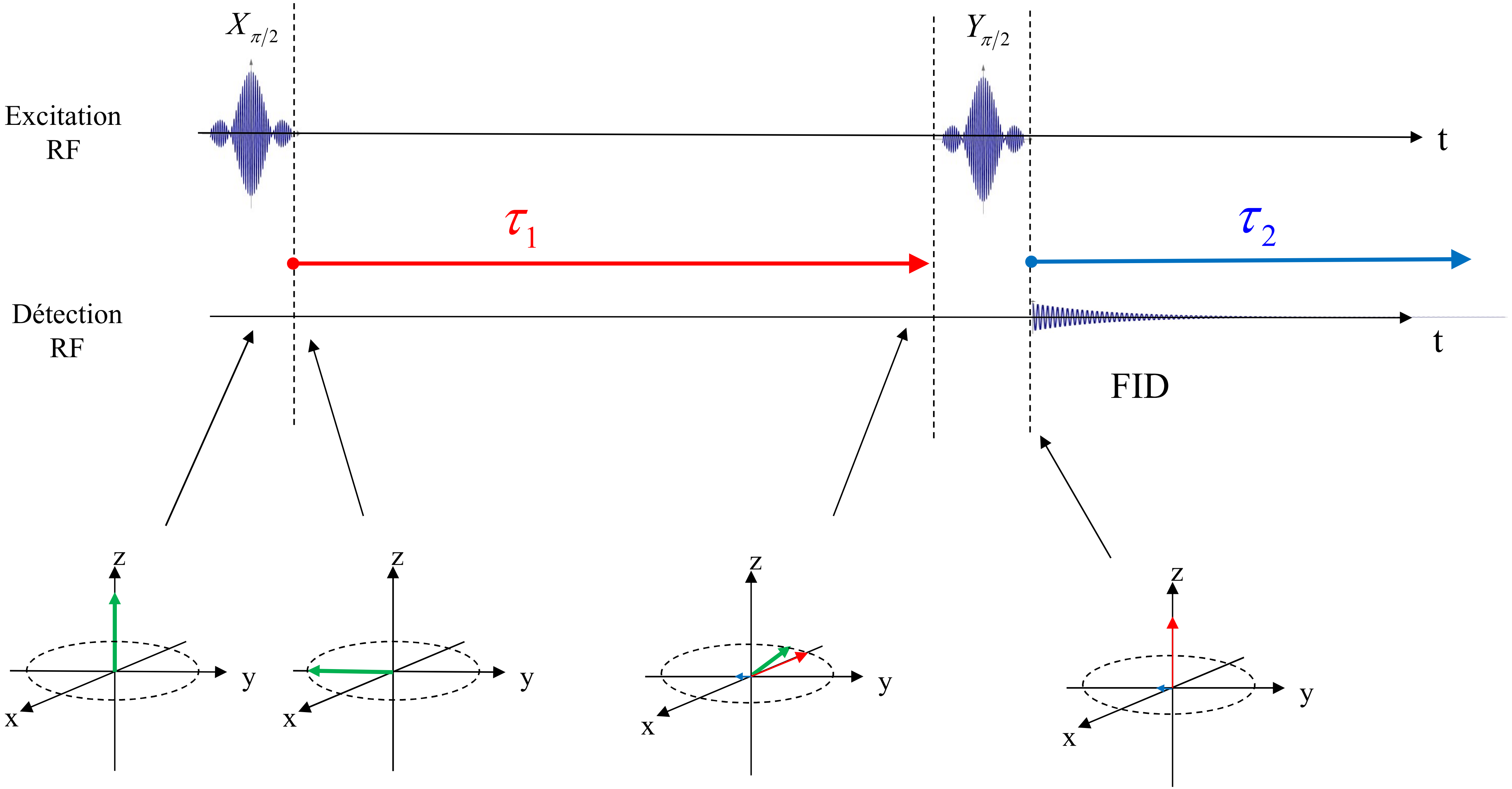




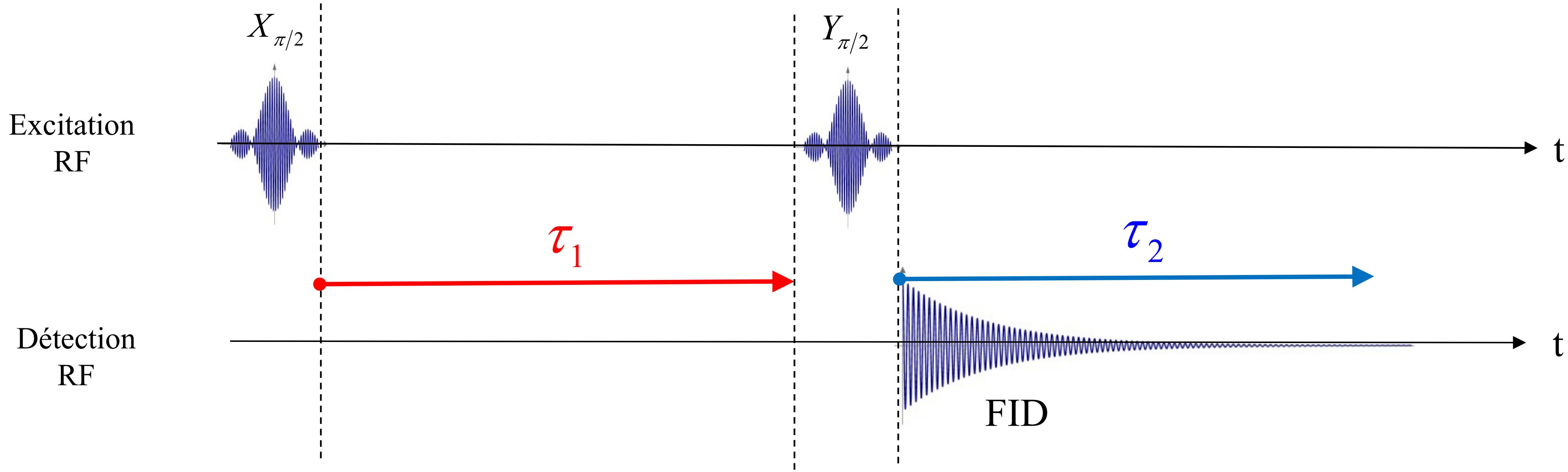
2D spectroscopie: exemple
COSY-90 (Correlated SpectroscopY)



2D spectroscopie: exemple
COSY-90 (Correlated SpectroscopY)



2D spectroscopie: exemple
COSY-90 (Correlated SpectroscopY)



$$\langle M_y(\tau_1,\tau_2)\rangle \cong e^{-i(\omega_1\cdot\tau_1)}\cdot e^{-i(\omega_2\cdot\tau_2)}$$

Fourier ⇩

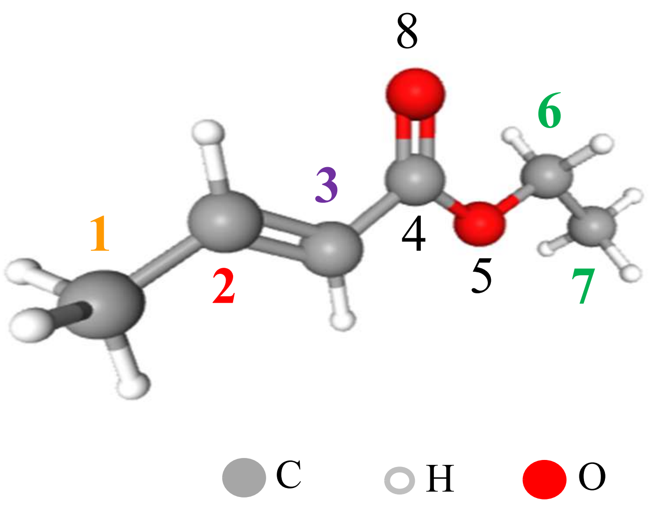
$$\langle \tilde{M}_y(\omega_1,\omega_2)\rangle$$

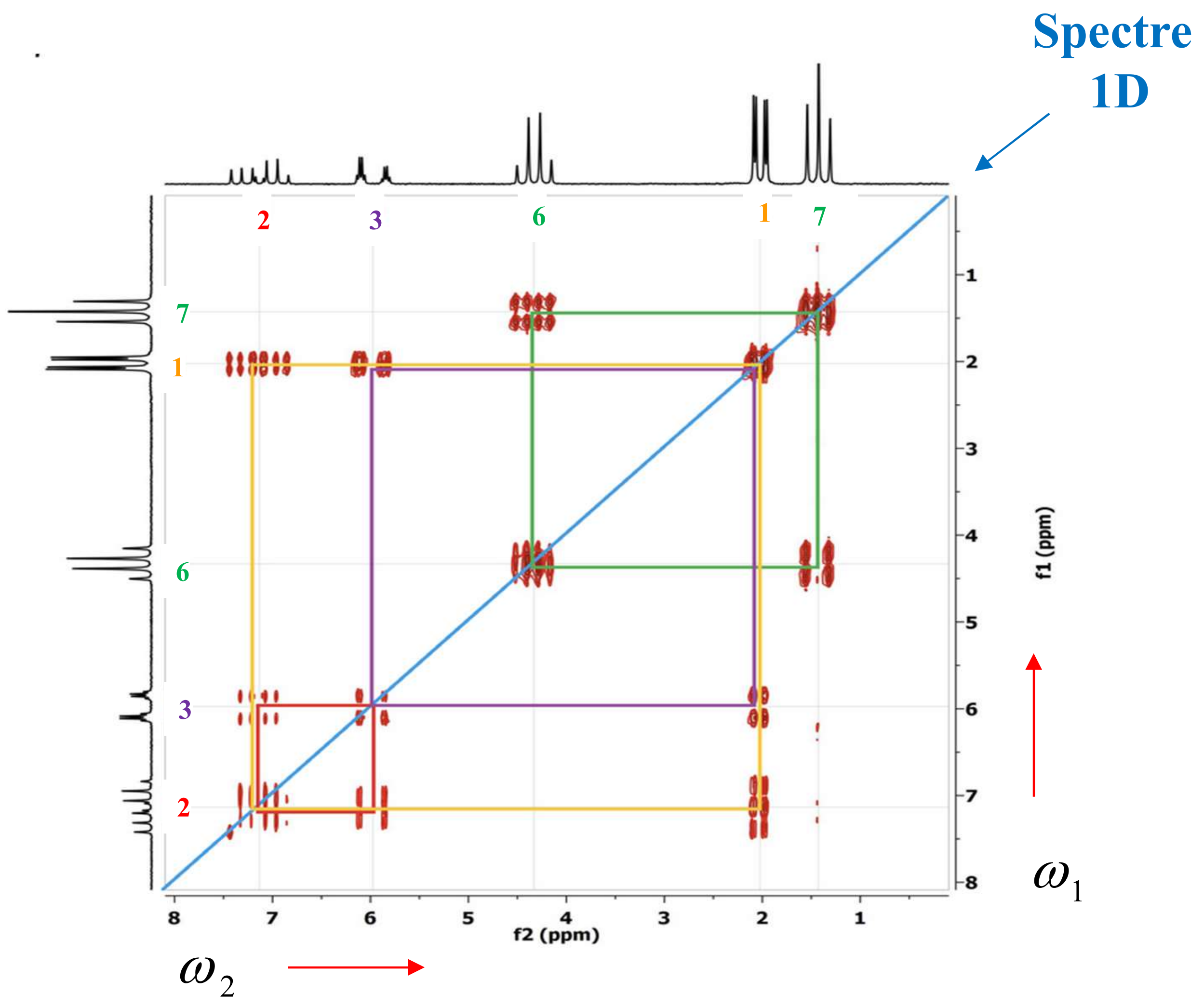
PAB

COSY-90: exemple

Ethyl crotonate

$C_6H_{10}O_2{=}C_3H_5\text{-}CO_2\text{-}C_2H_5$





Recherche des corrélations entre les spectres

→ Info sur la structure (couplages spin/spin)

http://www.qorganica.es/QOT/T12/COSY_int_e_exported/

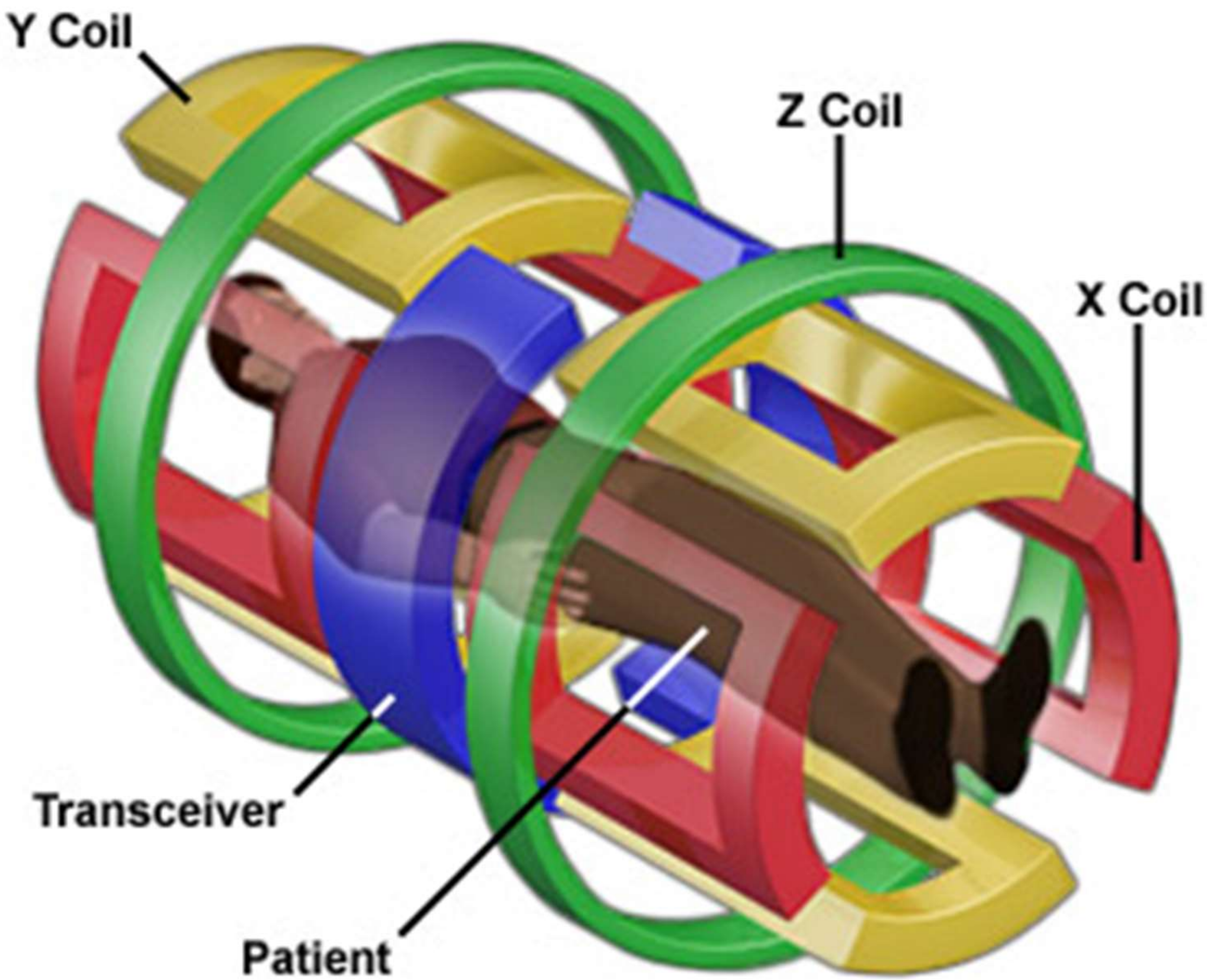
Imagerie par IRM

Spin local
des noyaux d'hydrogène

Scanner IRM

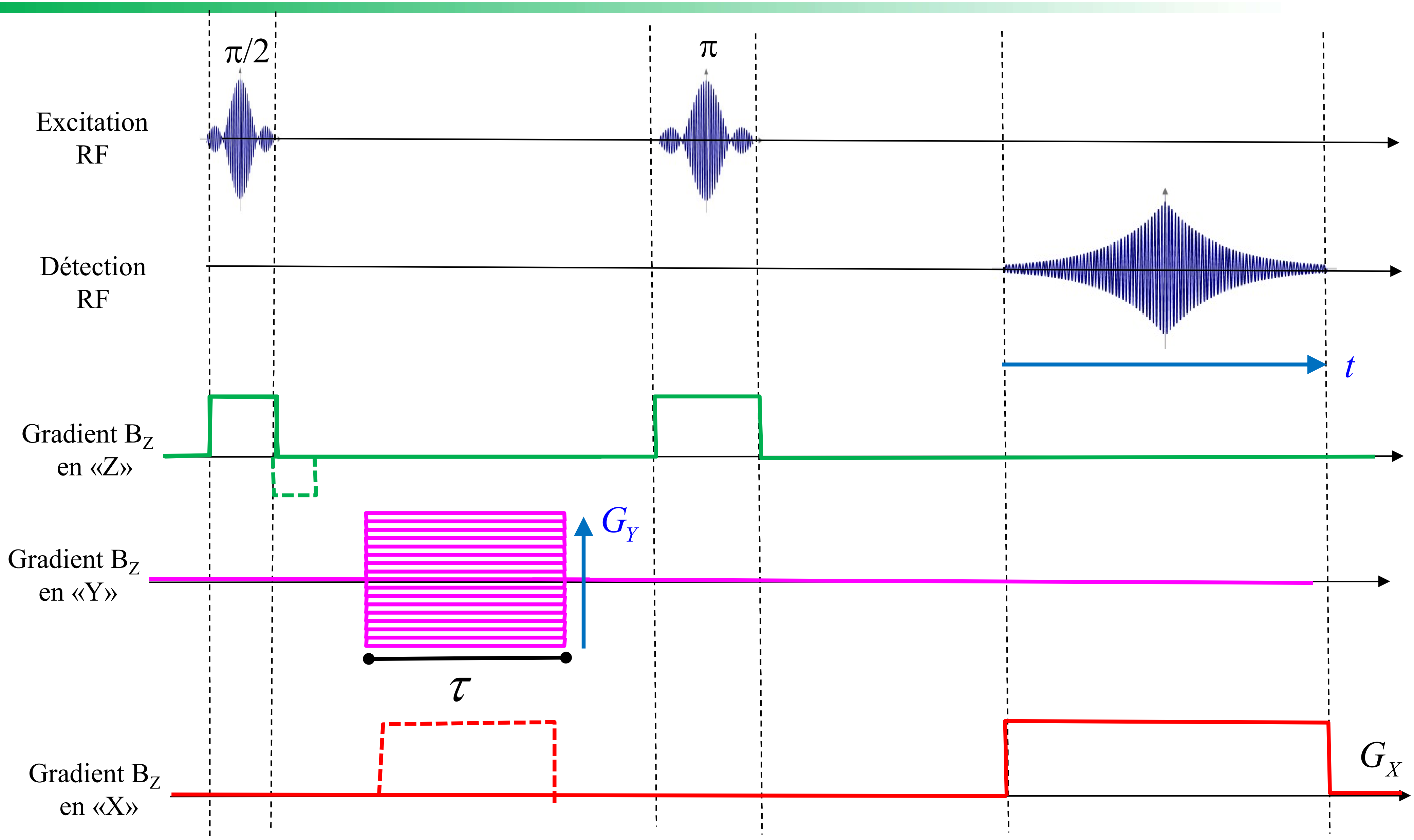
Besse PA, Klinik GUT St. Moritz

IRM: coils



https://www.researchgate.net/figure/MR-Scanner-Gradient-Coils-Source-http-wwwmagnetfsuedu_fig1_262494534

IRM: spin echo et gradients



IRM: reconstruction de l'image

Free Induction Decay (FID)

$$\varphi(t,G_Y)=\gamma\cdot B_Z(x)\cdot t+\gamma\cdot B_Z(y)\cdot\tau$$

$$\langle M_y(t,G_Y)\rangle\approx e^{i\varphi}$$

$$=\gamma\cdot(G_X\cdot x)\cdot t+\gamma\cdot(G_Y\cdot y)\cdot\tau$$

$$\langle M_y(K_X,K_Y)\rangle$$

$$=(\gamma\cdot G_X\cdot t)\cdot x+(\gamma\cdot\tau\cdot G_Y)\cdot y$$

$$\equiv K_X\cdot x+K_Y\cdot y$$

Image

Transformée de Fourier en K_X et K_Y

$$\langle\tilde{M}_y(x,y)\rangle$$

$$K_X\equiv(\gamma\cdot G_X\cdot t)$$

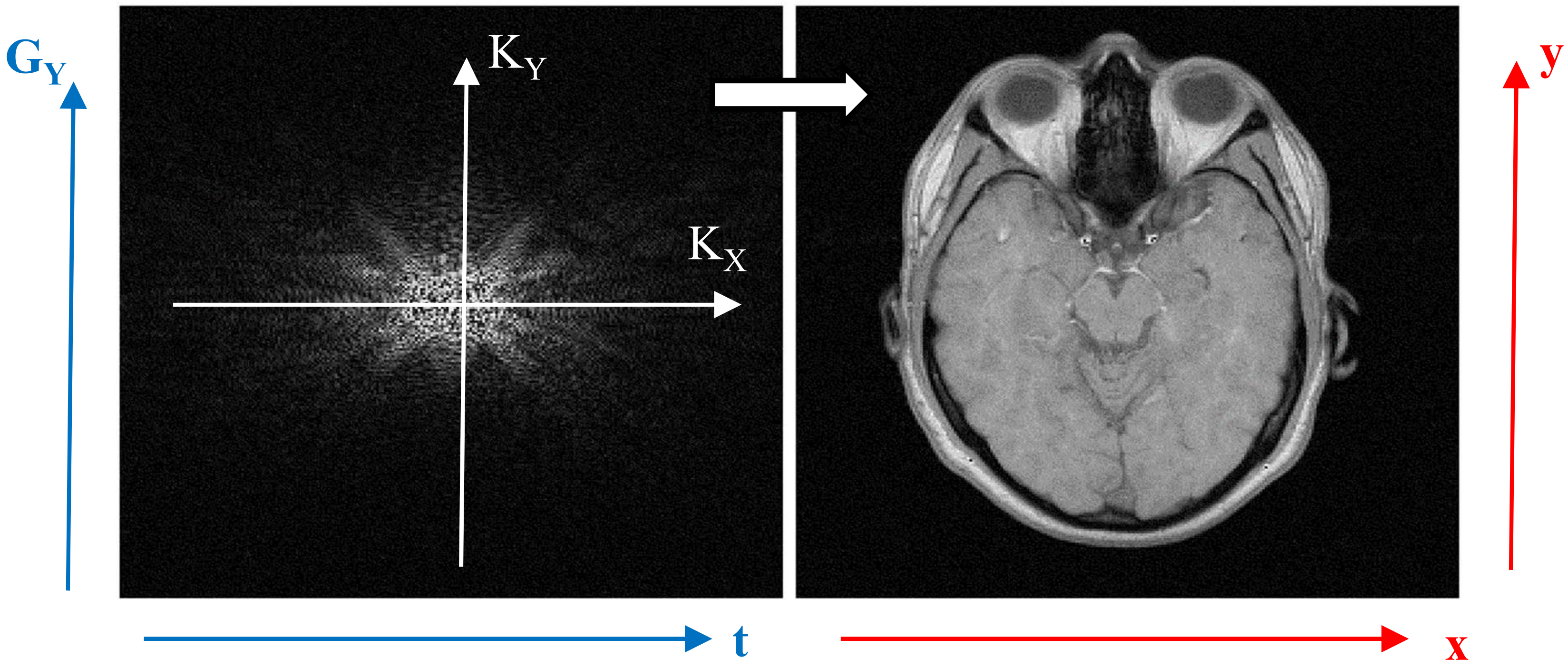
$$K_Y\equiv(\gamma\cdot\tau\cdot G_Y)$$

IRM: reconstruction de l’image

FID **Fourier** **Image**

$$\left\langle M_y(t, G_Y) \right\rangle = \left\langle M_y(K_X, K_Y) \right\rangle \Rightarrow \left\langle \tilde{M}_y(x, y) \right\rangle$$

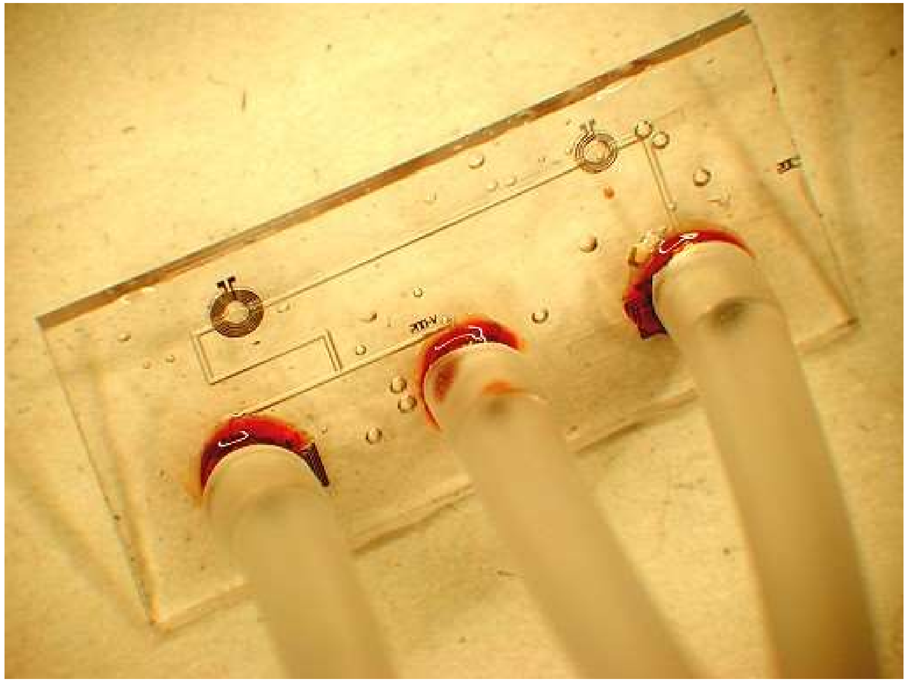
$K_X \equiv (\gamma \cdot G_X \cdot t)$ $K_Y \equiv (\gamma \cdot \tau \cdot G_Y)$



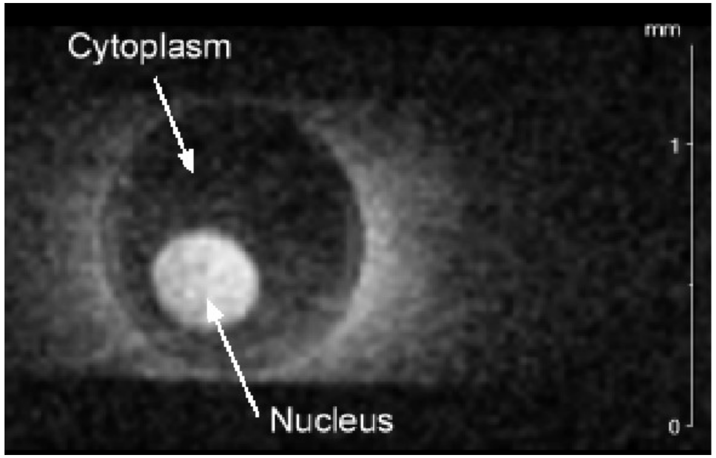
https://compphys.go.ro/nuclear-magnetic-resonance-and-fourier-transform/

NMR et IRM on chip

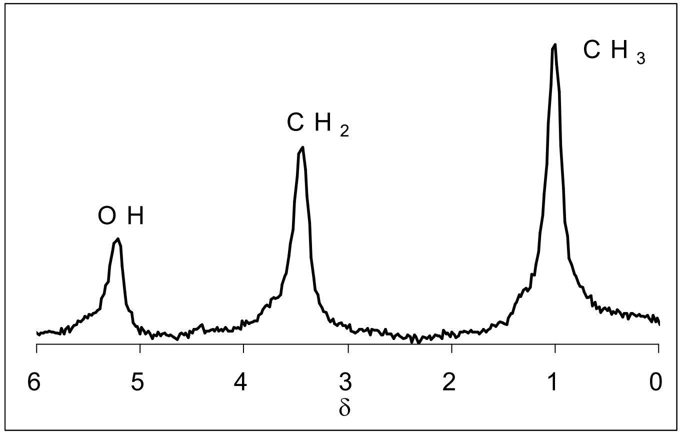
Ch. Massin et al. LMIS3 - EPFL



IRM: ovocyte de grenouille



NMR: 30nL Ethanol CH_3CH_2OH

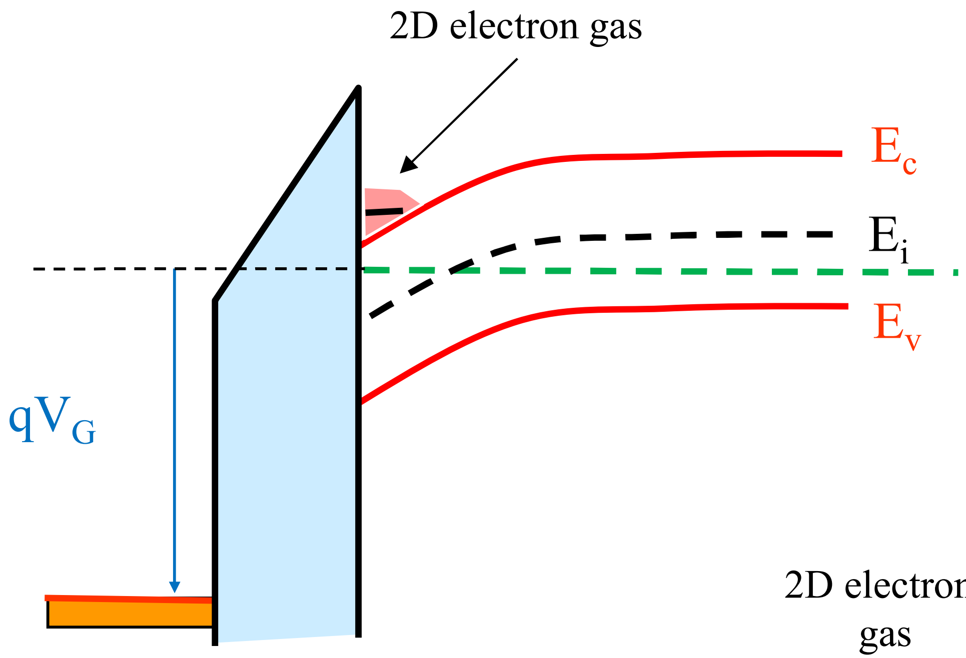


Electronic Spin Qubits

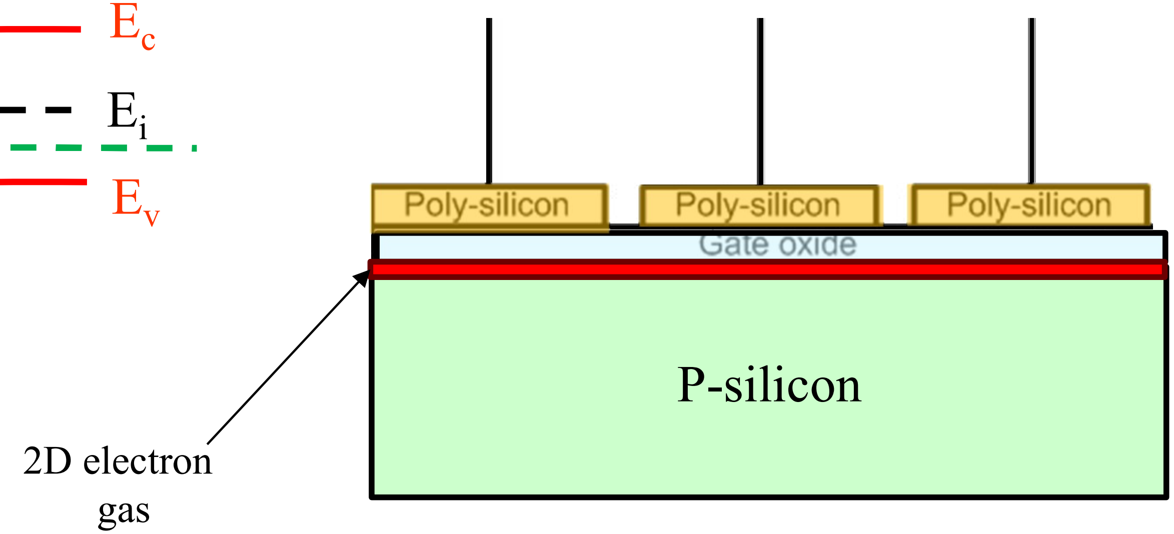
Structure et quantum box

Structure MOS:
gaz électronique 2D

NMOS structure

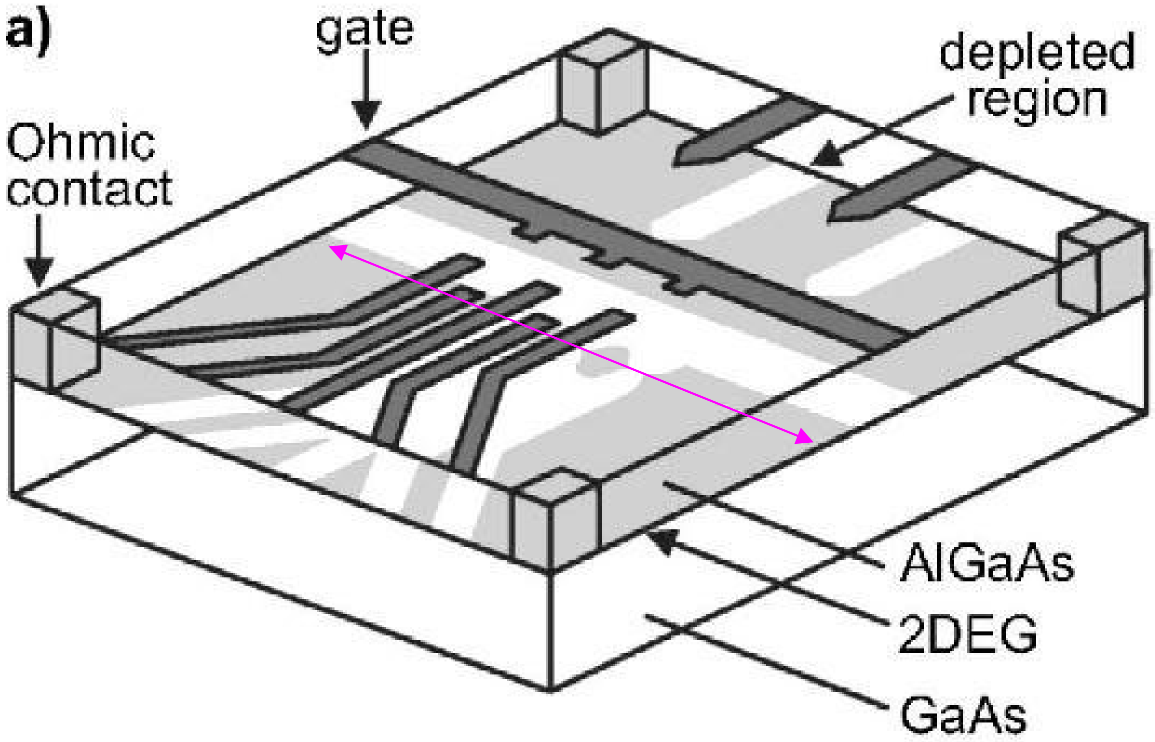


CCD register

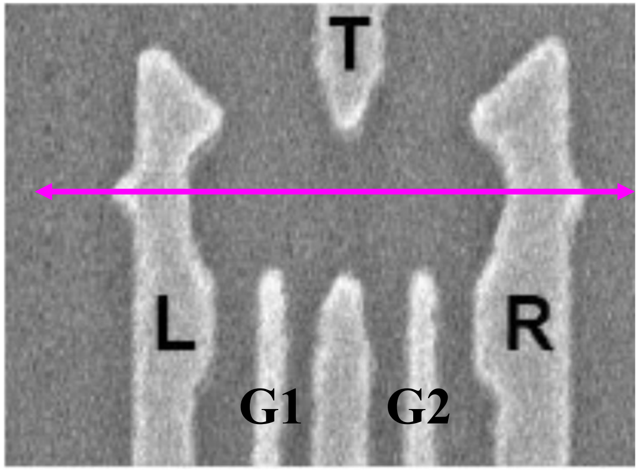


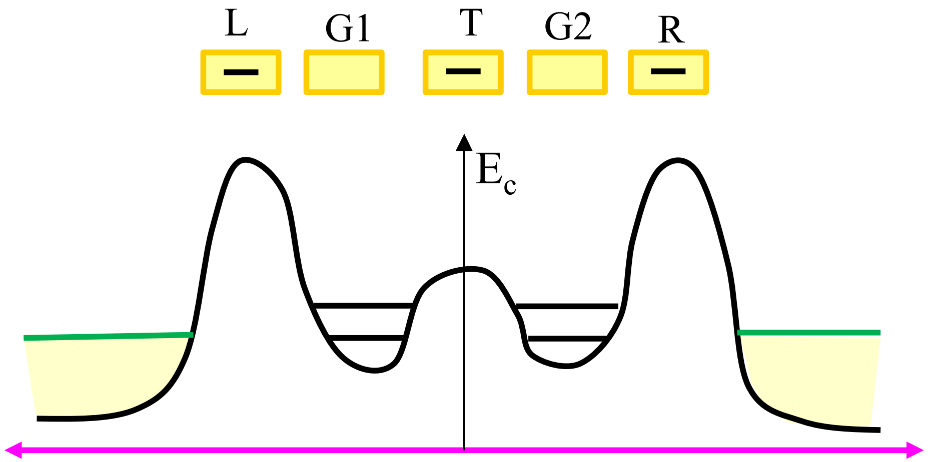
Paire de spin qubits

https://www.science.org/doi/10.1126/science.1116955

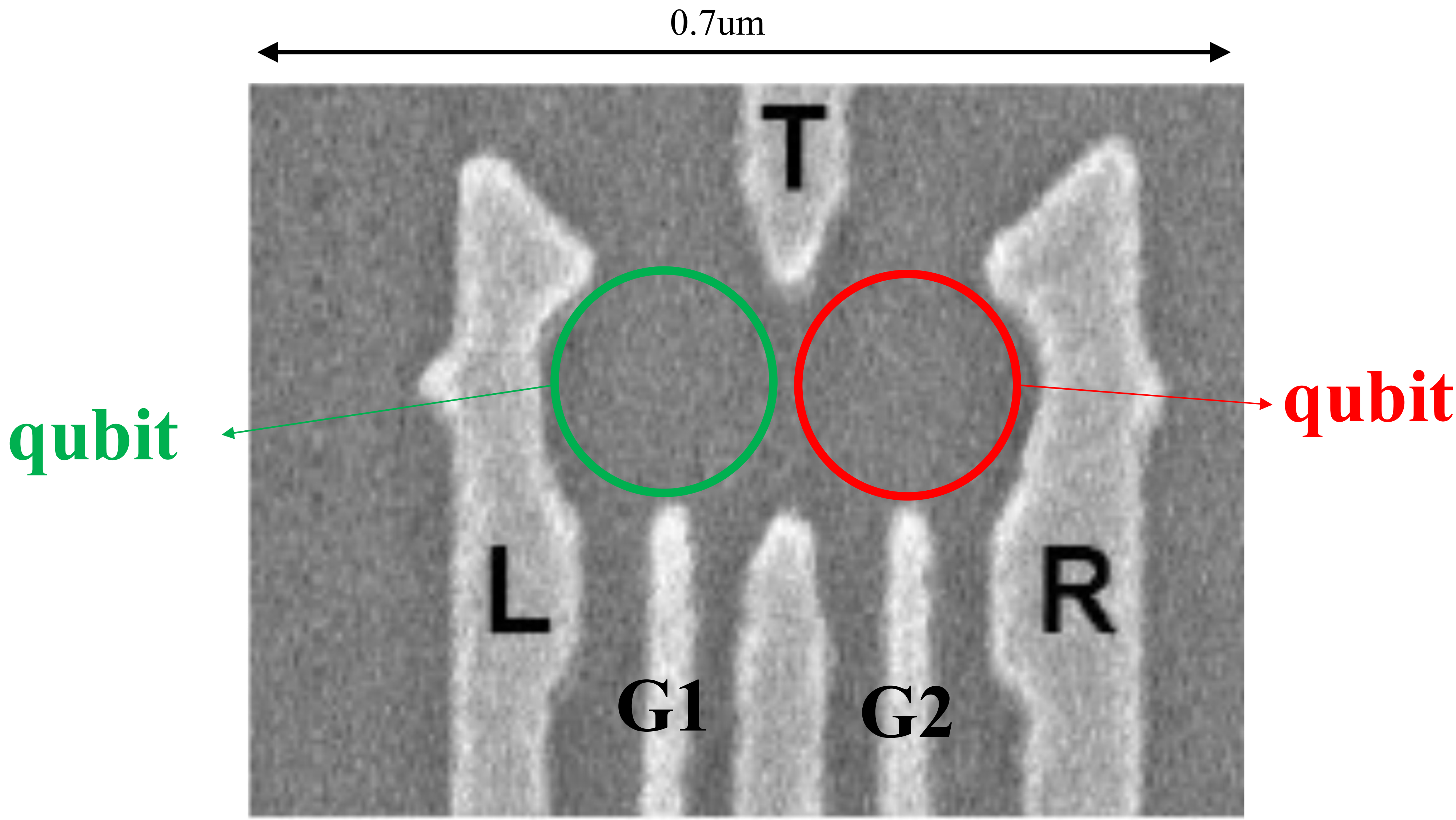


https://www.semanticscholar.org/paper/Simulating-Charge-Stability-Diagrams-for-Double-and-Powell/9ad8a90e1ecfc4269638b774fcf27c7b0544ecc5



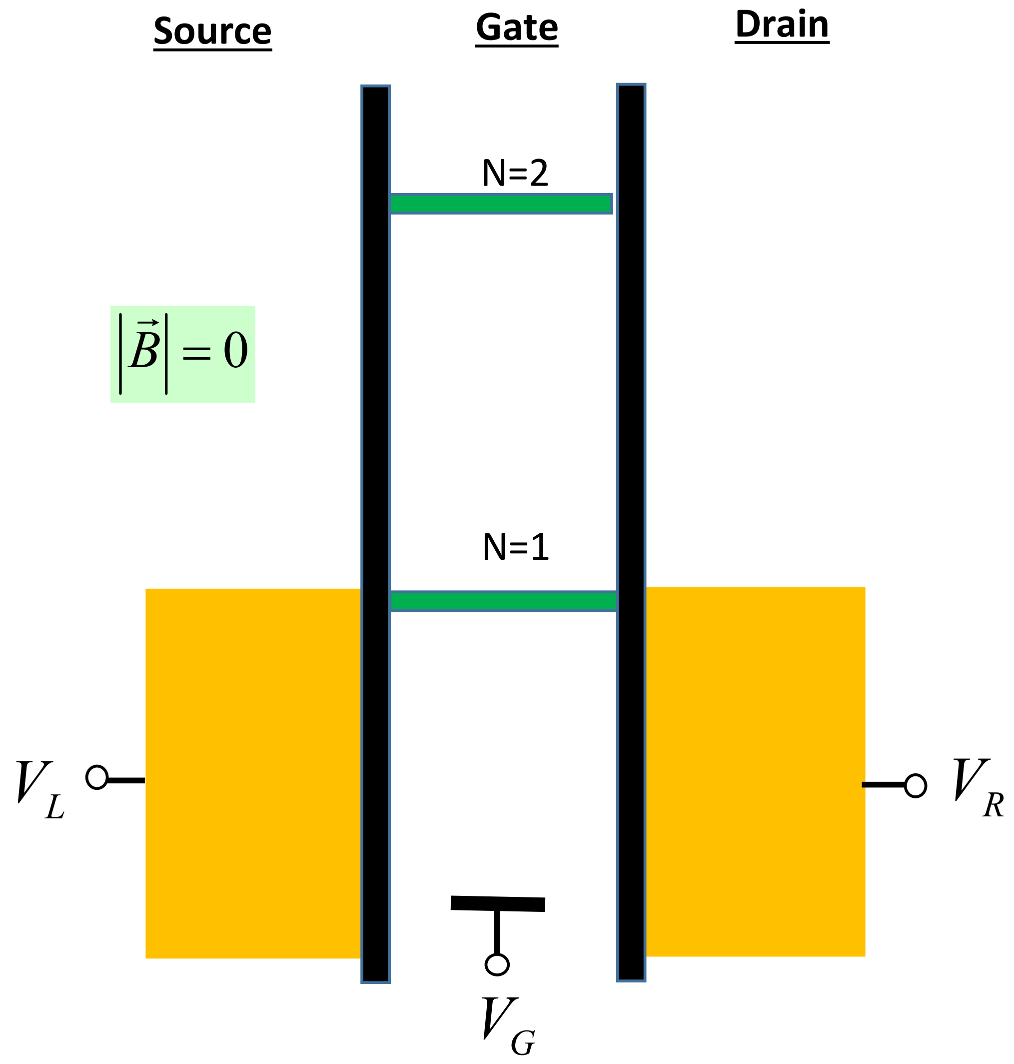


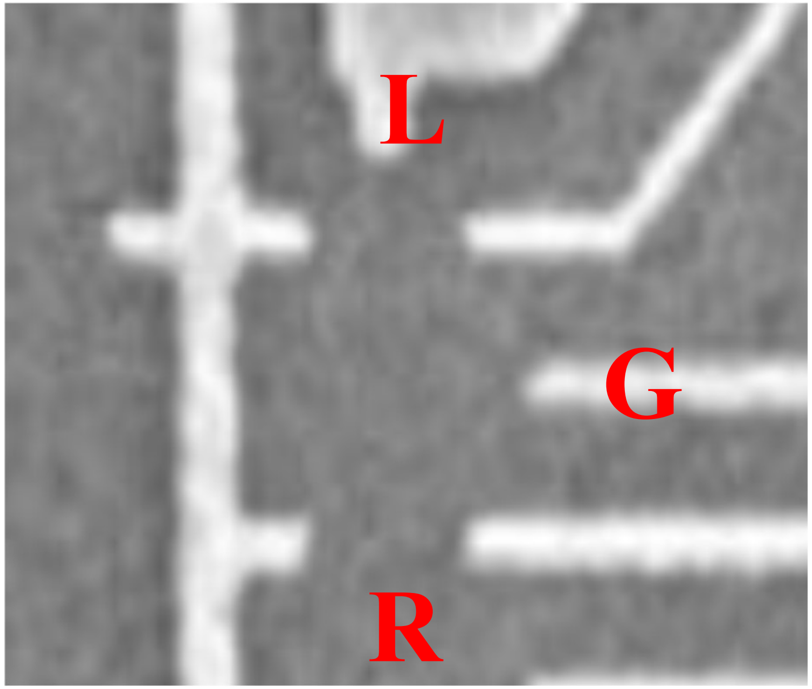
Two coupled spin Qubits



https://www.science.org/doi/10.1126/science.1116955

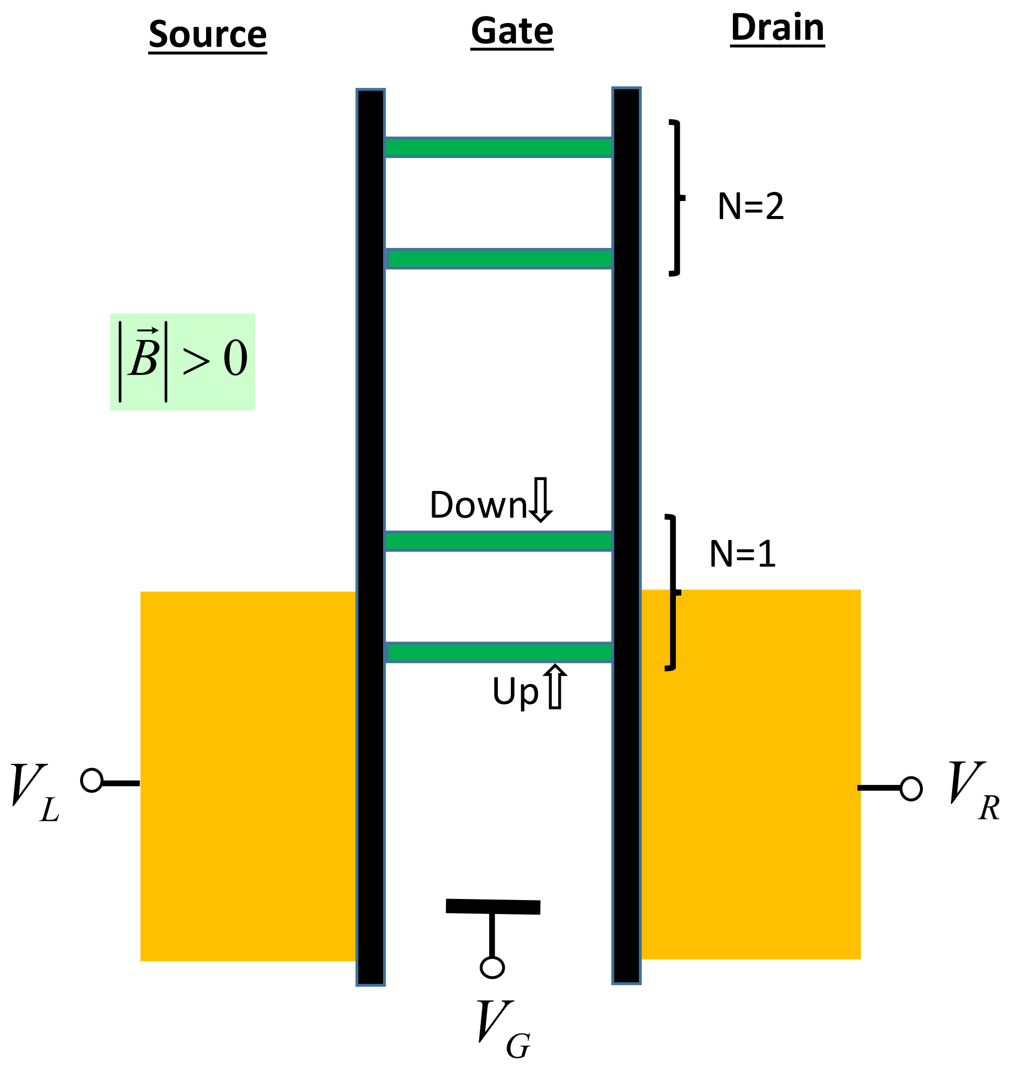
Quantum box sans champ magnétique

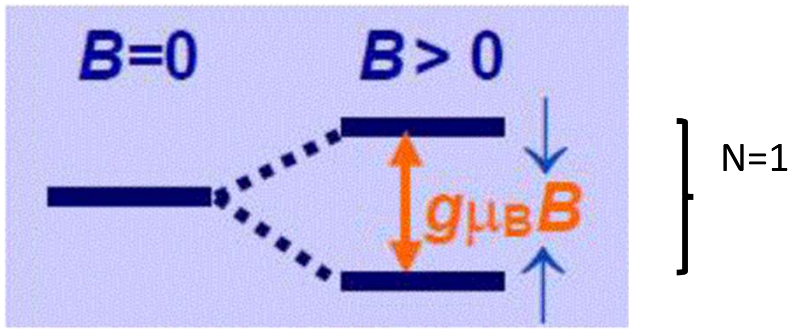




https://qutech.nl/wp-content/uploads/2019/01/2005__Elzerman2005_Chapter_SemiconductorFew-ElectronQuant.pdf

Quantum box dans un champ magnétique



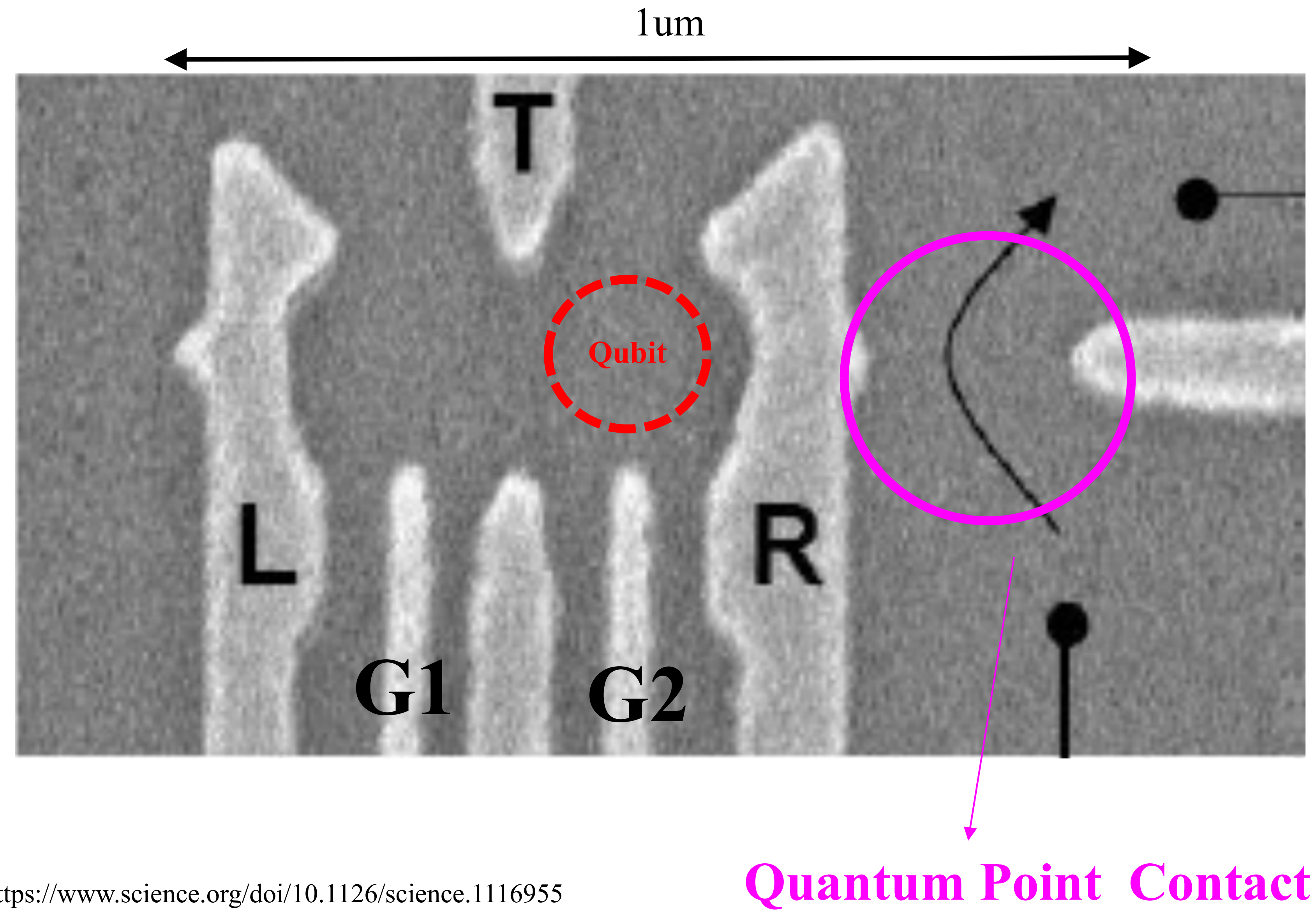


$$\omega = g \cdot u_B \cdot |B| \;\cong 38\left[\tfrac{GHz}{T}\right] \cdot |B|$$

avec $g = 0.44$ $\qquad \mu_B \equiv \dfrac{q}{2m_e}$

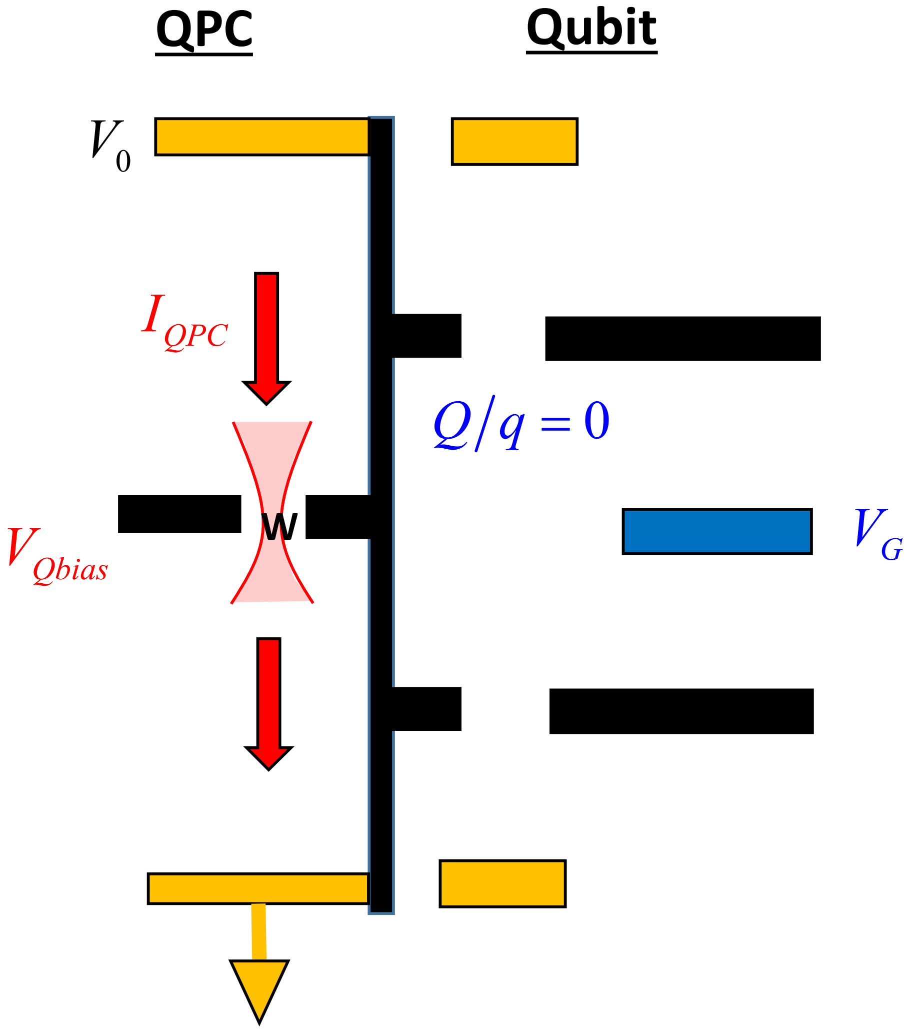
Electronic Spin Qubits
Mesures par
quantum point contact

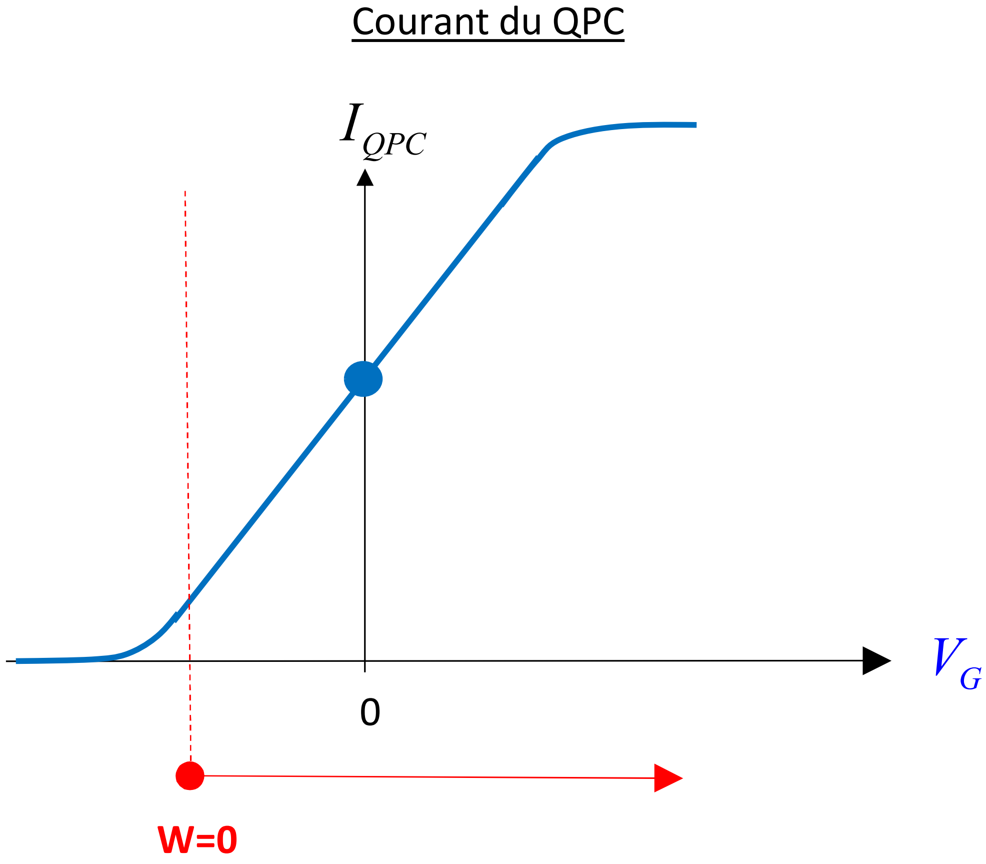
Quantum Point Contact



https://www.science.org/doi/10.1126/science.1116955

Quantum Point Contact (QPC)

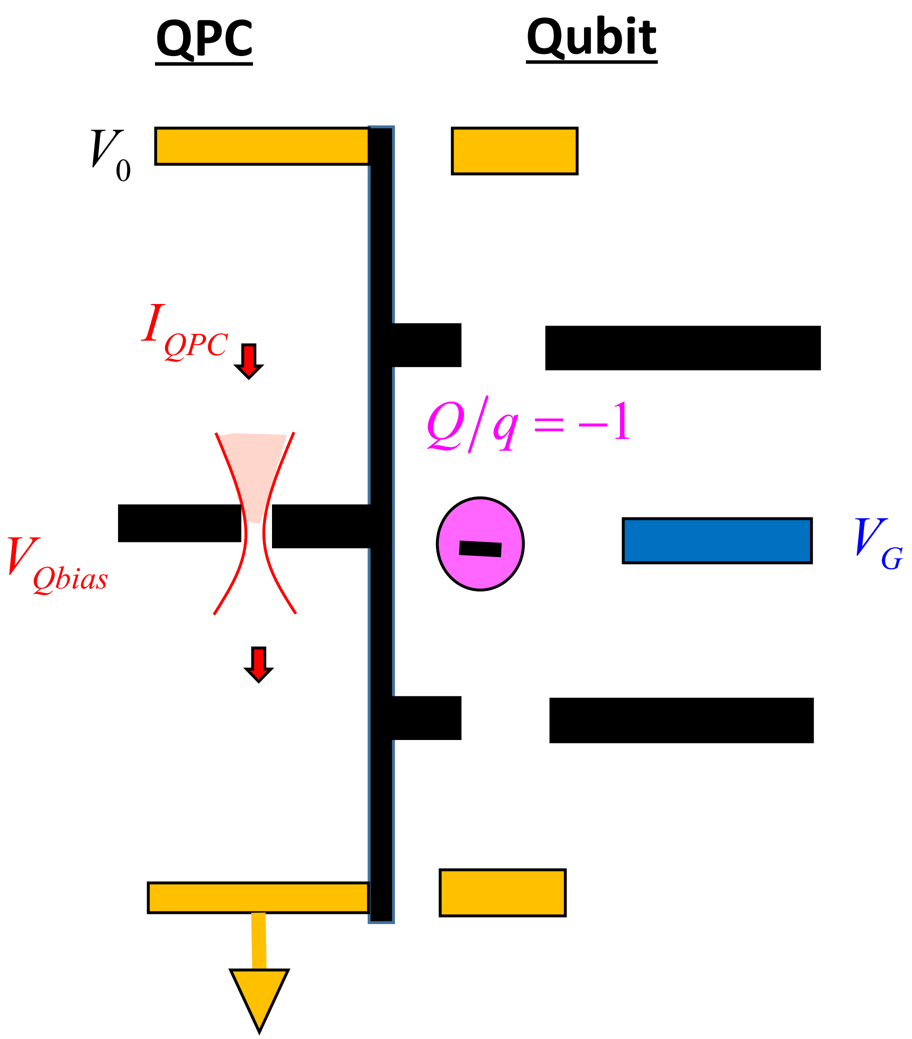


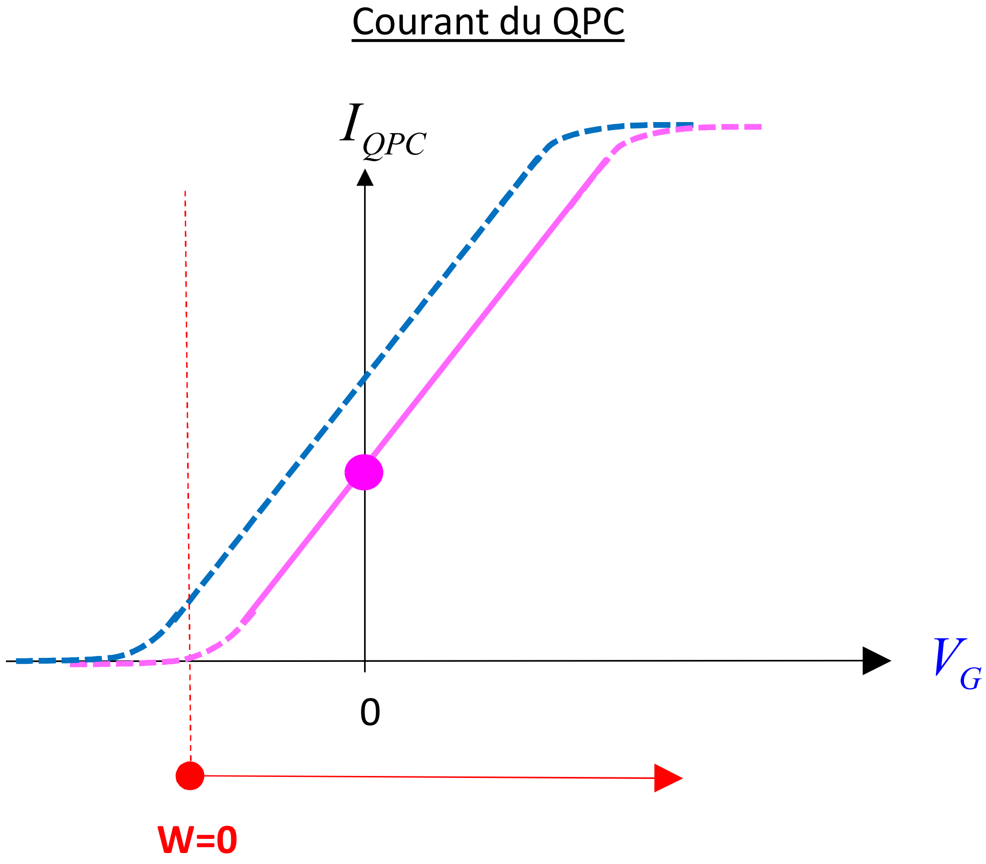


Courant: $I_{QPC} = G(V_G) \cdot V_0$

«Quantum non-demolition»

Quantum Point Contact (QPC)

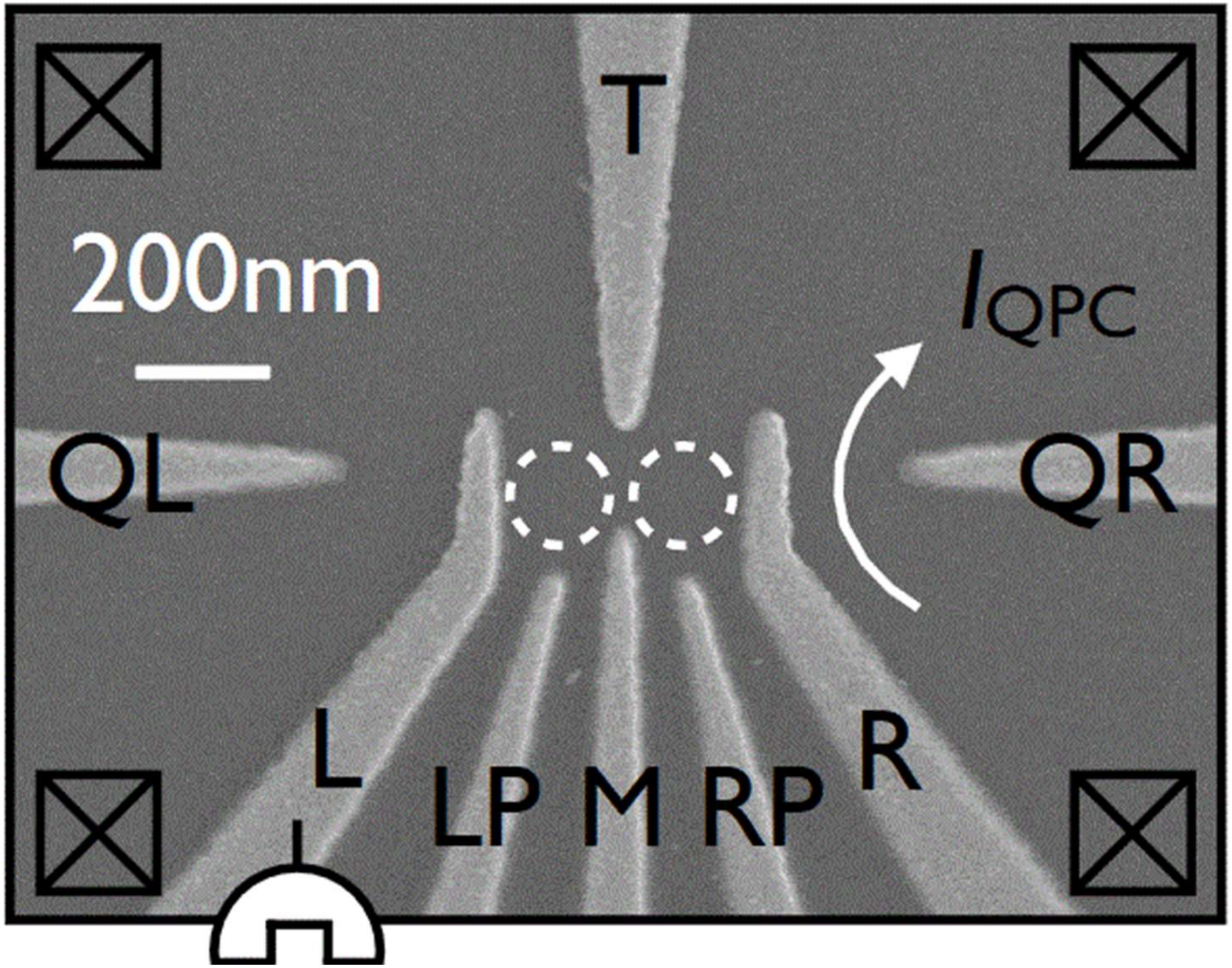




Courant: $I_{QPC} = G(V_G) \cdot V_0$

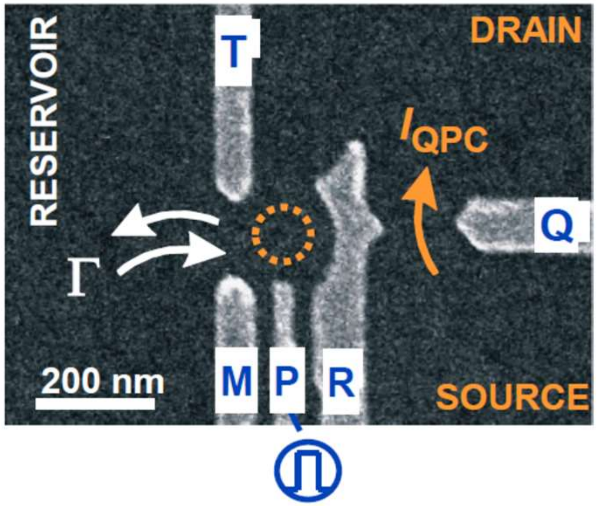
«Quantum non-demolition»

Quantum Point Contact



https://arxiv.org/pdf/1401.4416.pdf

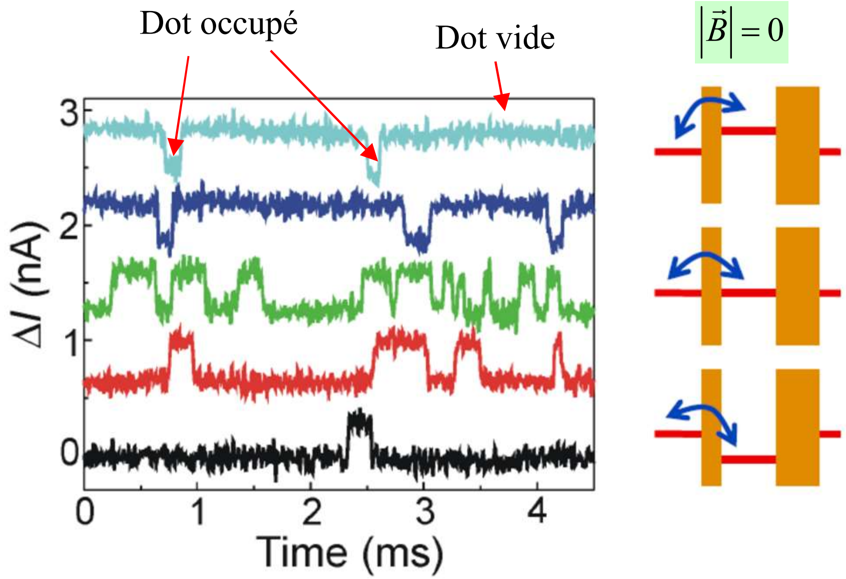
Spin qubit



- V_{SD} = 1 mV
- I_{QPC} ~ 30 nA
- ΔI_{QPC} ~ 0.3 nA
- Shortest steps ~ 8 µs

See single electrons jump on/off the dot in real-time

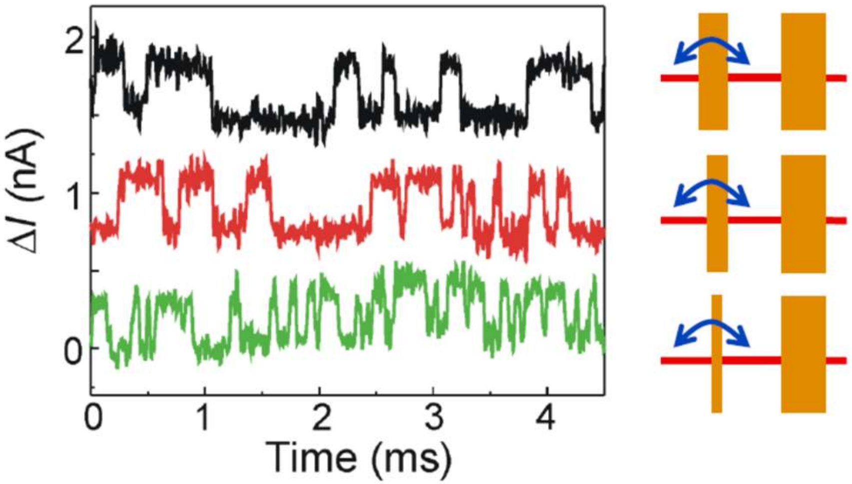
Vandersypen et al, APL 2004



Dot rarement occupé

Nombreux échanges

Dot souvent occupé



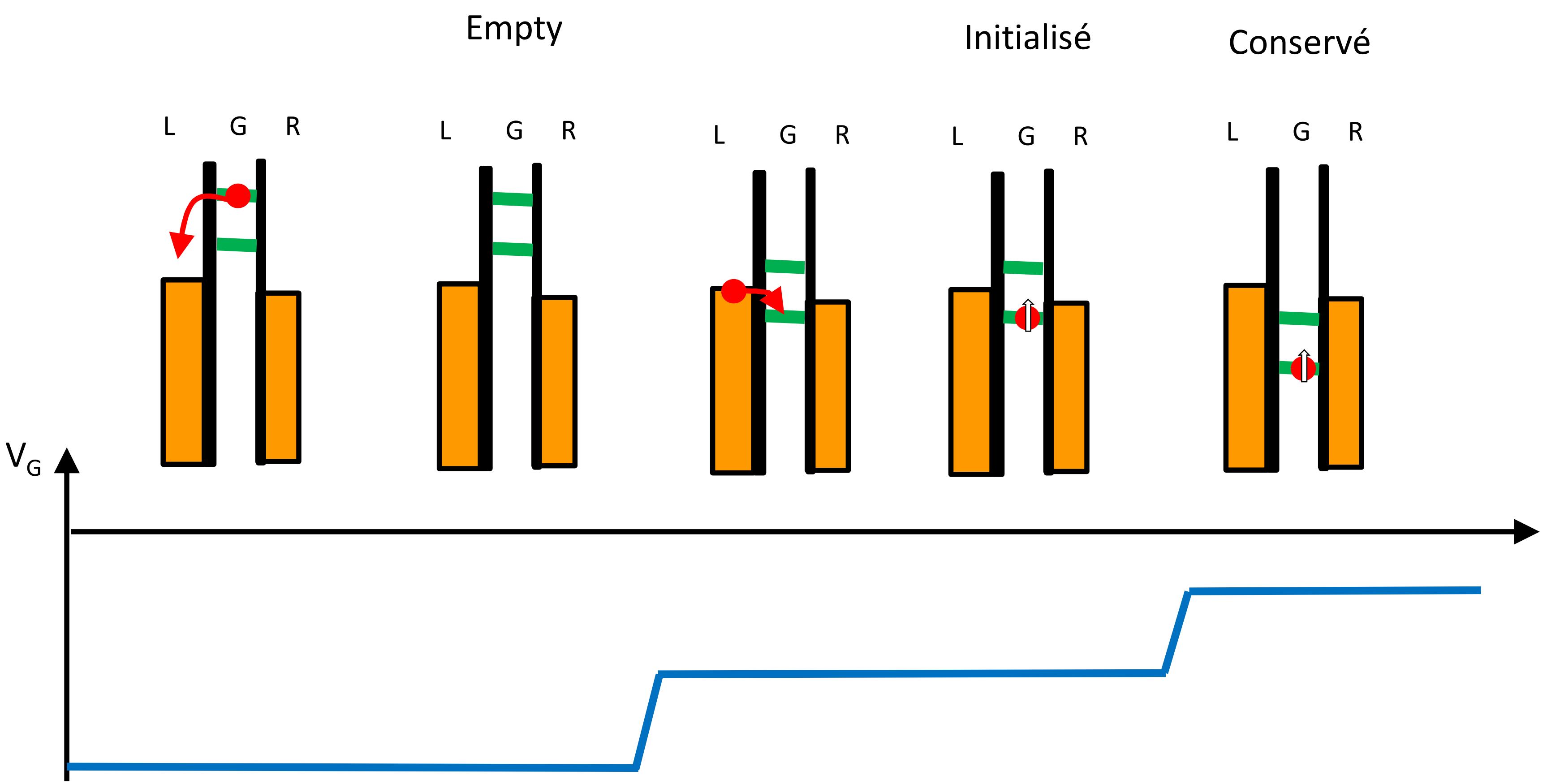
Large barrière
peu d'échanges

Faible barrière
Nombreux échanges

Electronic Spin Qubits

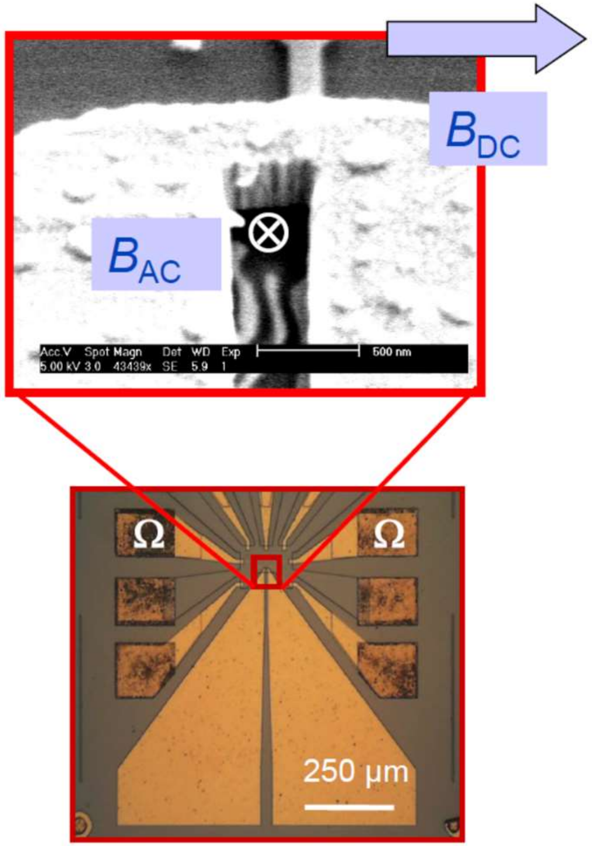
Initier et manipuler

Spin qubit: Initier et conserver



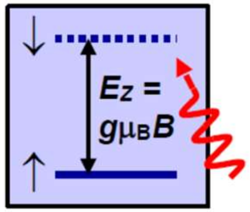
Manipuler par des champs magnétiques HF

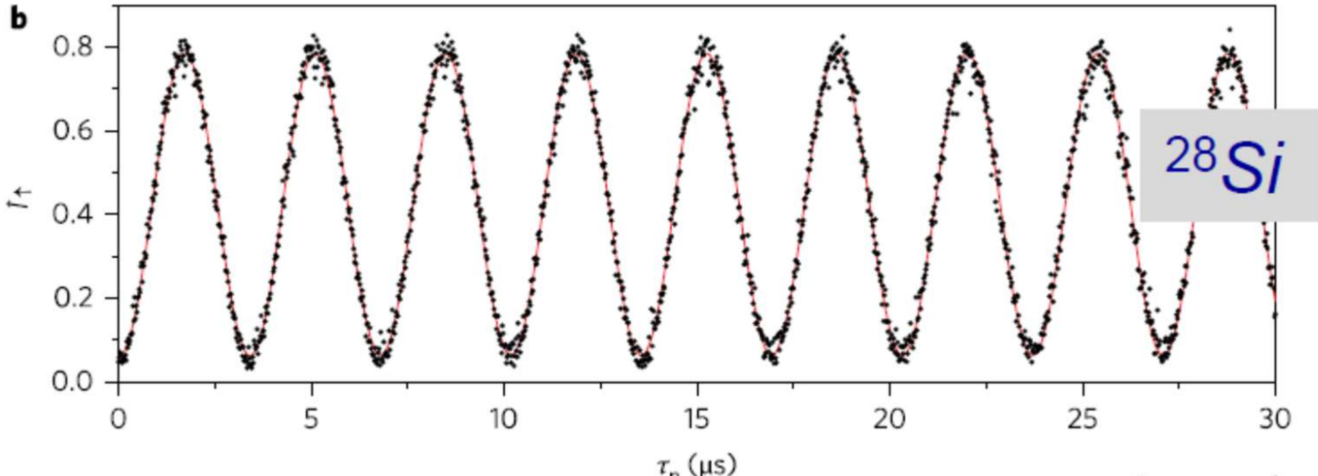
$$H_m = -\frac{\hbar\gamma}{2}\cdot\left(B_{Z0}\cdot\sigma_Z + B_X(\omega)\cdot\sigma_X\right)$$



ESR — pulsed microwave magnetic field

$H_{RF} \sim \Sigma\, A_i(t)\cos(\omega_i t)\;\sigma_{xi}$





Rabi

Veldhorst et al, Nature Nano 2014

Electronic Spin Qubits

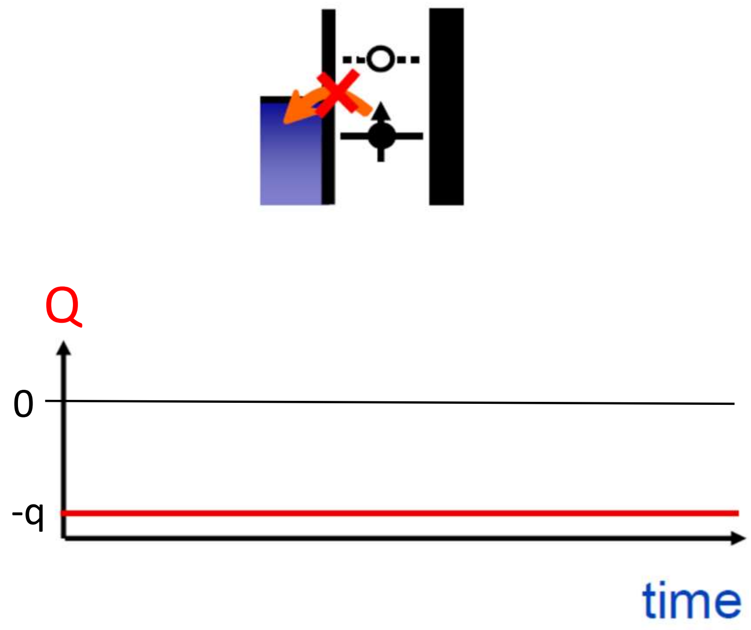
Détecter

Readout: «signature» Up / Down

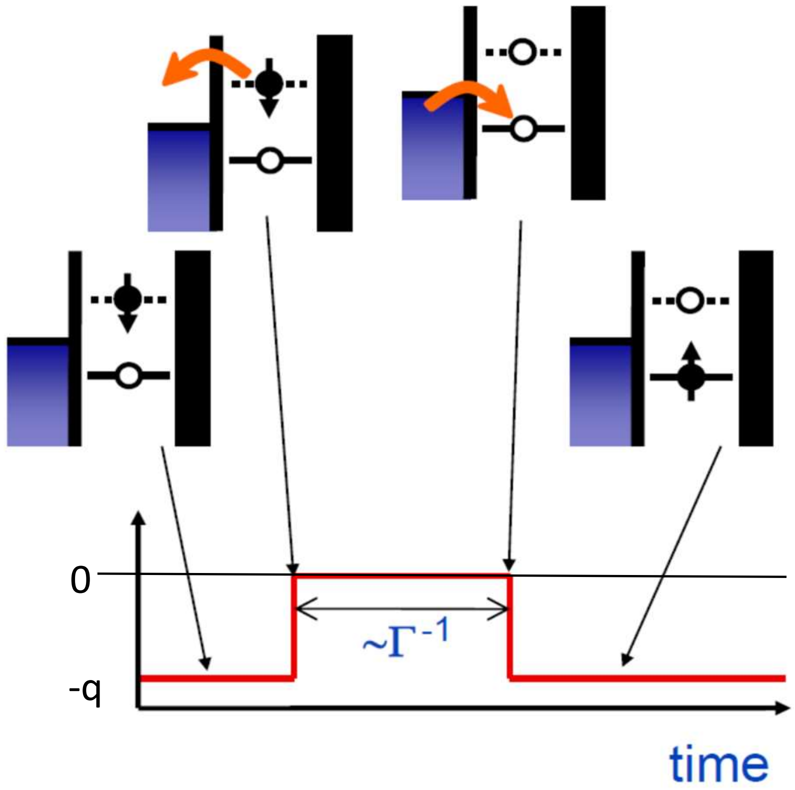
Transformer le «spin Up», «spin Down» en état de charge dans le quantum dot

Spin Up

↓ and ↑ split due to high magnetic field

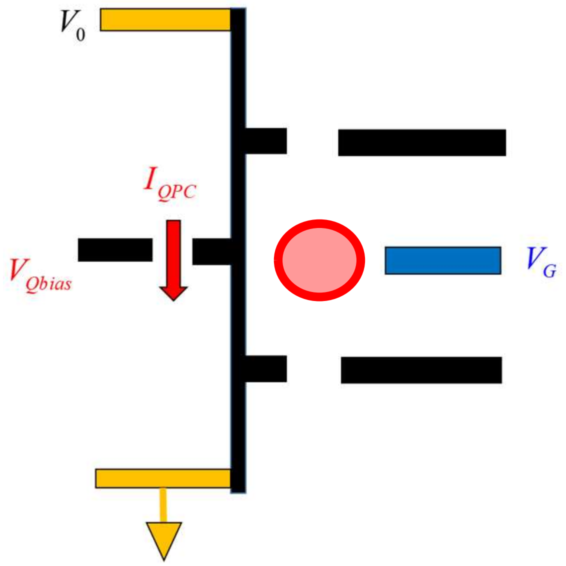


Spin Down

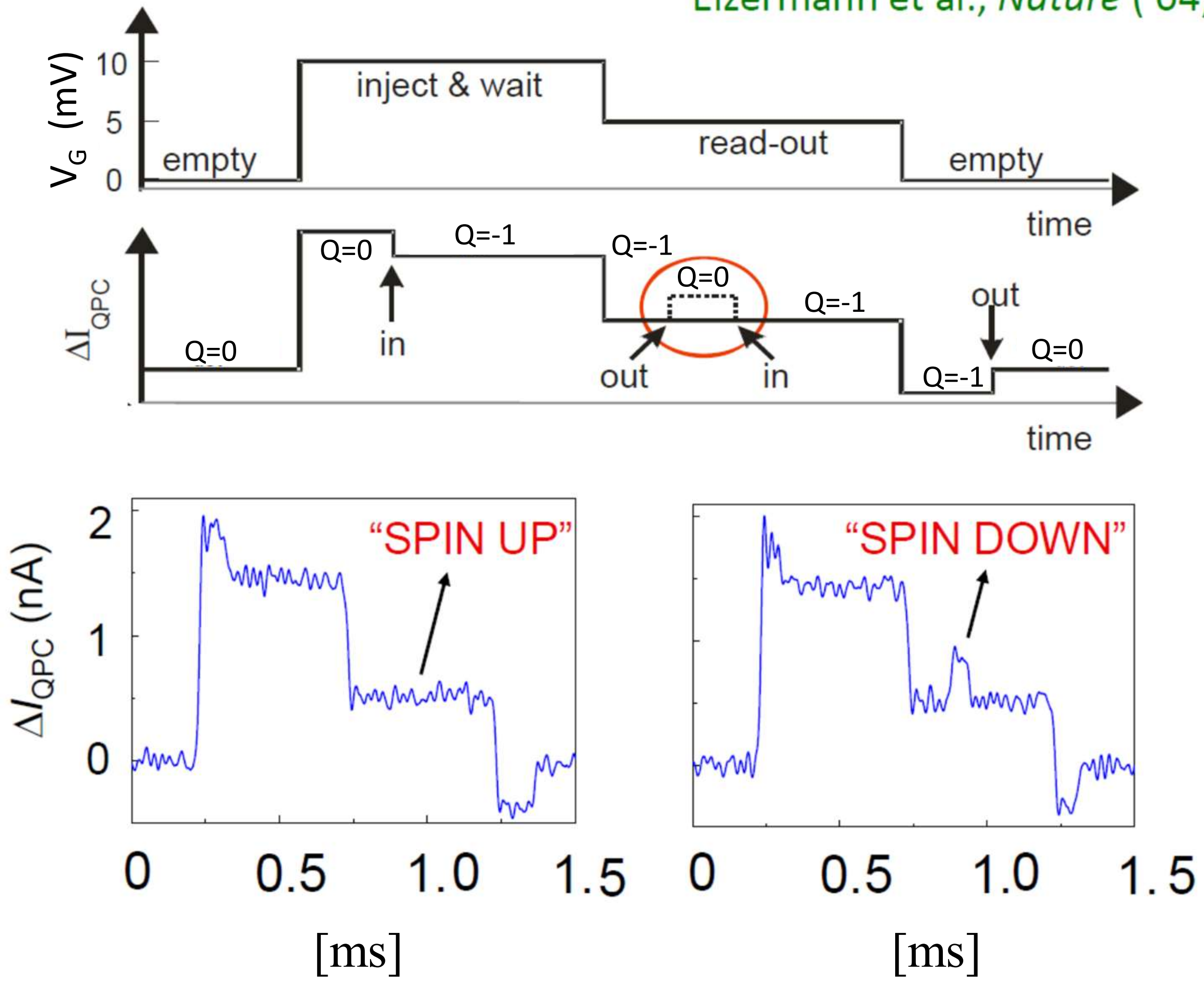


Elzermann et al., *Nature* ('04)

Readout: quantum point contact et «signature»



Elzermann et al., *Nature* ('04)



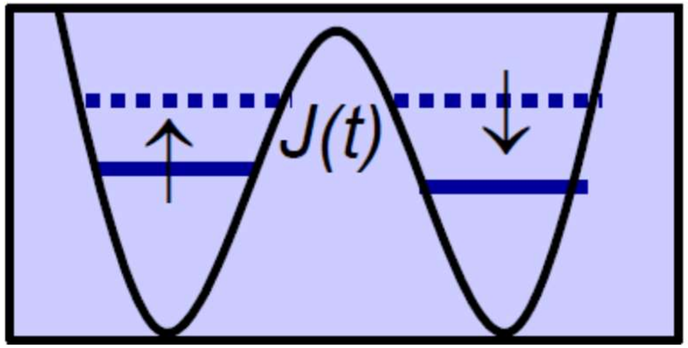
Paire et chaine d’ Electronic Spin Qubits

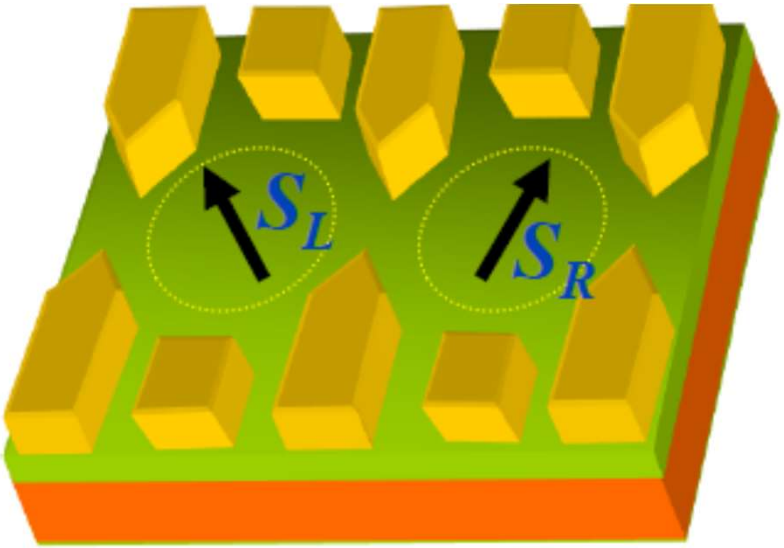
Couplage de spin qubits

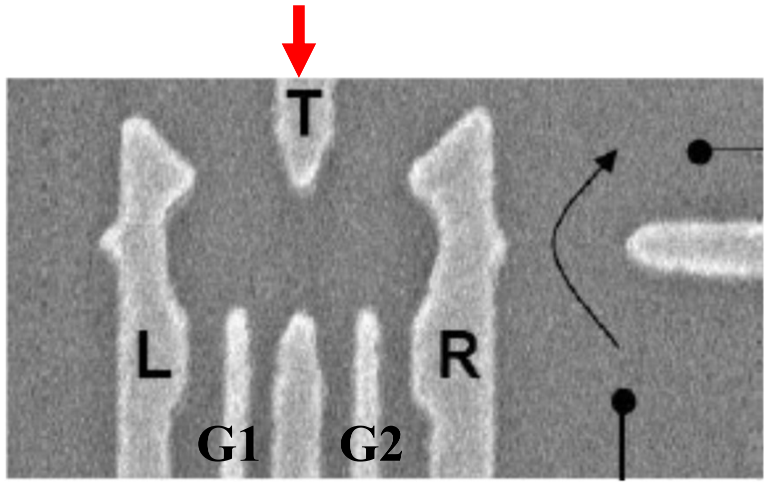
$$\sqrt{SWAP}$$

exchange interaction

$$H_J \sim \Sigma\, J_{ij}(t)\ \vec{\sigma}_i \cdot \vec{\sigma}_j$$



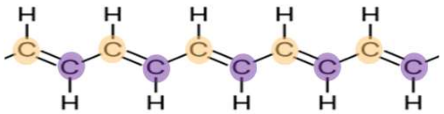


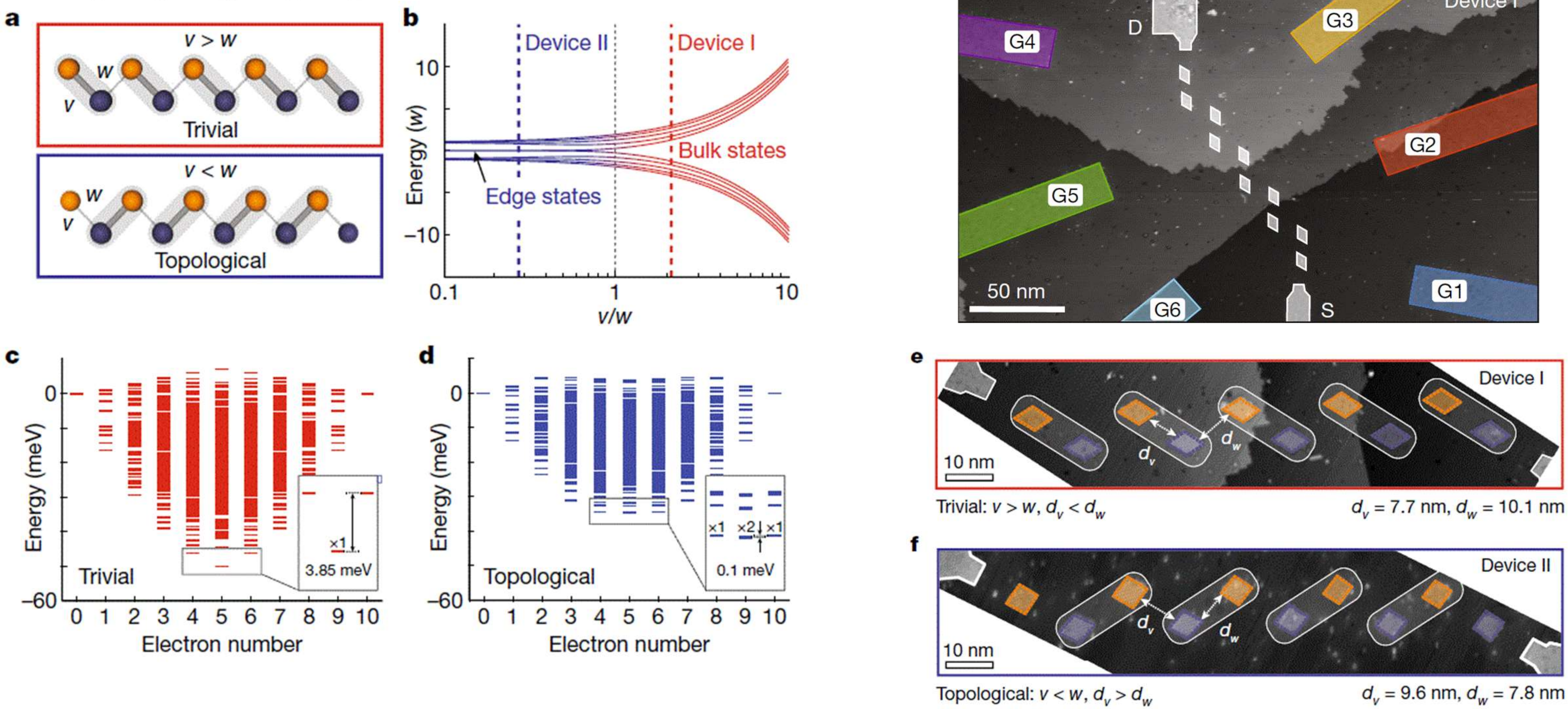


https://en.wikipedia.org/wiki/Spin_qubit_quantum_computer

https://www.science.org/doi/10.1126/science.1116955

Simulations chimiques: polyacétylène





M. Kiczynski et al, «Engineering topological states in atom-based semiconductor quantum dots», Nature | Vol 606 | 23 June 2022, pp. 694-699, https://doi.org/10.1038/s41586-022-04706-0


Bonne pause et bonnes révisions