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COLLEGE ON

PHYSICS OF NANO-DEVICES

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An introduction to magnetic resonance in quantum information processing

Presented by:

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An introduction to magnetic resonance in quantum information processing

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Bits

Information: 0 or 1

Classical 2-state systems:

- capacitor (charged/uncharged)
- bistable transistor network
- polarization of magnetic domain
- ...

Qubits

Information: $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$

Quantum 2-state systems (proposals):

- charge states
- photon polarizations
- flux states (superconductors)
- spin states
- ...

Bit logic

Classical NOT
(1 bit gate):

Input	Output
0	1
1	0

Classical CNOT
(2 bit gate):

Inputs		Output
0	0	0
0	1	1
1	0	1
1	1	0

Qubit logic

Quantum CNOT (2 qubit gate):

$$\begin{aligned} |\psi\rangle &= \alpha_0 |\downarrow\downarrow\rangle + \alpha_1 |\downarrow\uparrow\rangle + \alpha_2 |\uparrow\downarrow\rangle + \alpha_3 |\uparrow\uparrow\rangle \\ &\equiv \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} \end{aligned}$$

$$\mathcal{U}_{\text{CNOT}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\mathcal{U}_{\text{CNOT}} \left(\frac{|\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle}{\sqrt{2}} \right) = \left(\frac{|\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle}{\sqrt{2}} \right)$$

Quantum single qubit gates: $\mathcal{R}$

Outline of lectures

First part:

- Magnetic resonance tutorial
- General aspects of application to quantum information

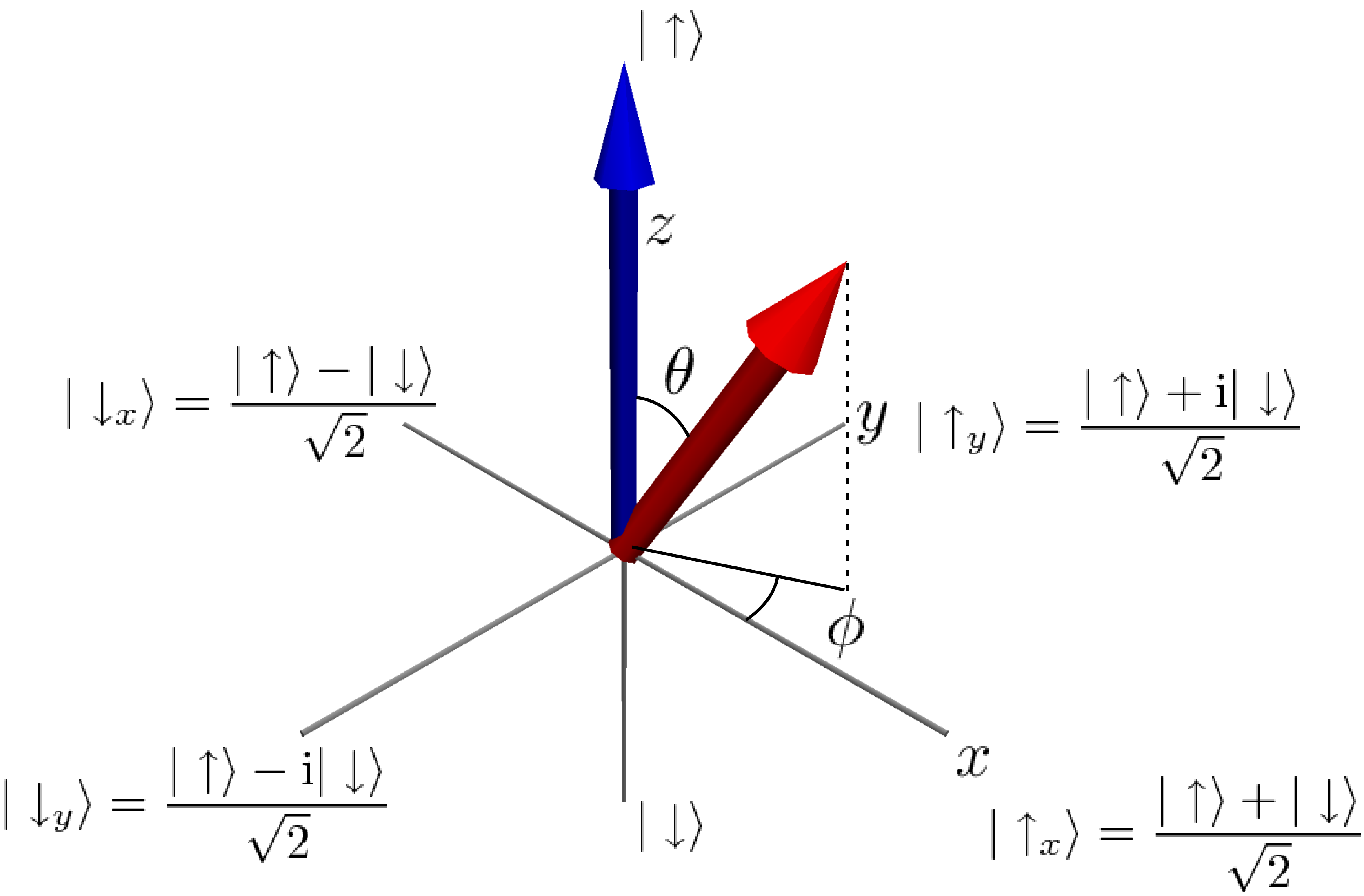
Second part:

- $N@C_{60}$
- Using ESR for qubit manipulation

Things not covered, but interesting anyway!

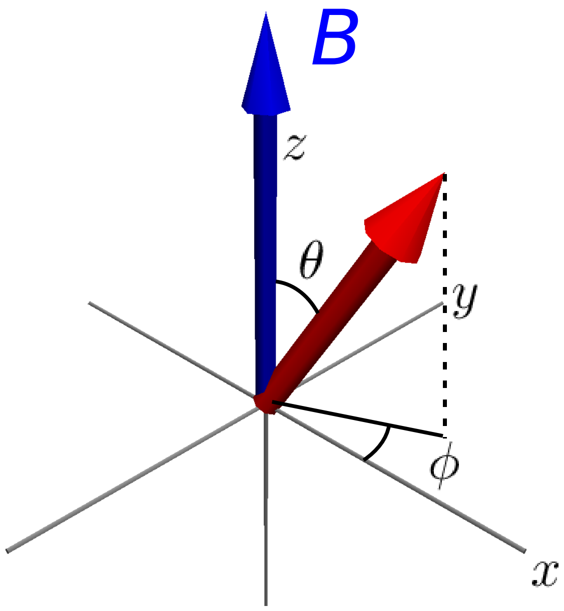
Bloch sphere

$$|\psi\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(\mathrm{i}\phi)\sin(\theta/2)|\downarrow\rangle$$



Precession

$$|\psi\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(\mathrm{i}\phi)\sin(\theta/2)|\downarrow\rangle$$



With magnetic field *B* along *z*,

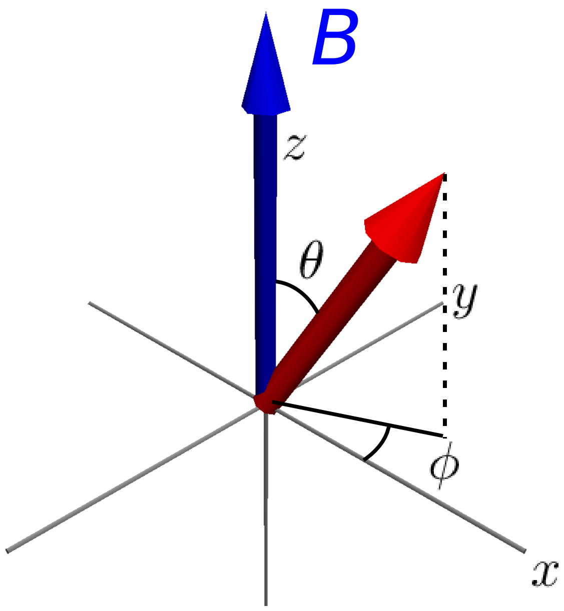
$$\begin{aligned} E(|\uparrow\rangle) &= \frac{1}{2}g\mu B = \frac{1}{2}\hbar\omega \\ E(|\downarrow\rangle) &= -\frac{1}{2}g\mu B = -\frac{1}{2}\hbar\omega \end{aligned}$$

where $\omega = g\mu B/\hbar$

$$\begin{aligned} |\psi(t)\rangle &= \exp\left(-\mathrm{i}\frac{\omega t}{2}\right)\cos(\theta/2)|\uparrow\rangle + \exp\left(\mathrm{i}\left(\phi + \frac{\omega t}{2}\right)\right)\sin(\theta/2)|\downarrow\rangle \\ &= \exp\left(-\mathrm{i}\frac{\omega t}{2}\right)\left[\cos(\theta/2)|\uparrow\rangle + \exp\left(\mathrm{i}(\phi + \omega t)\right)\sin(\theta/2)|\downarrow\rangle\right] \end{aligned}$$

Precession

$$|\psi\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(\mathrm{i}\phi)\sin(\theta/2)|\downarrow\rangle$$



For a general field along ϑ, φ,

$$\mathcal{H}|\psi\rangle = \frac{1}{2}\hbar\omega\sigma|\psi\rangle = \mathrm{i}\hbar\frac{\partial}{\partial t}|\psi\rangle$$

with

$$\sigma = \sin\vartheta\cos\varphi\;\sigma_x + \sin\vartheta\sin\varphi\;\sigma_y + \cos\vartheta\;\sigma_z$$

$$|\psi(t)\rangle = \exp\left(-\mathrm{i}\frac{\omega t}{2}\sigma\right)|\psi(0)\rangle$$

$$\exp\left(\hat{A}\right) = I + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \cdots$$

1-qubit problem solved?

Arbitrary rotations possible using finite-duration magnetic fields

Technical problems:

- application of dc fields for short durations; stray fields
- measurement of state of a single spin
- selectivity
- ...

Magnetic resonance offers a methodology

Magnetic resonance

Apply static field (B_0) → precession

Apply oscillatory field (B_1)

- circularly polarized
- on resonance with moment
- transverse to static field

→ resonance

Work in rotating frame

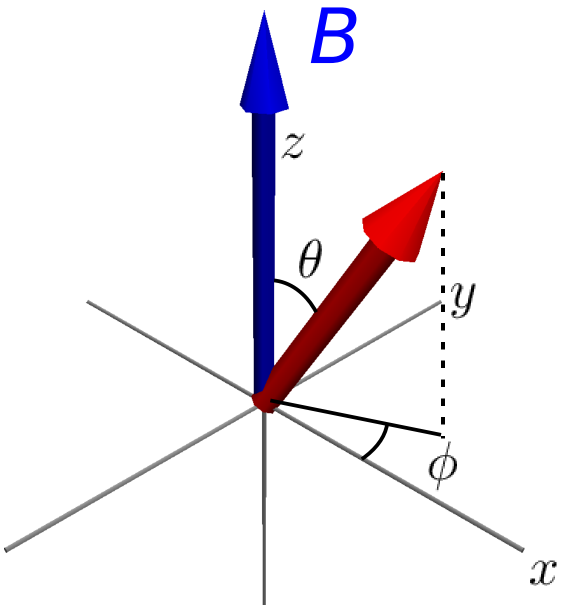
→ consider only transverse fields (on resonance)

Do experiment simultaneously on many identical systems

→ macroscopically measurable response

Relaxation, decoherence

$$|\psi\rangle = \cos(\theta/2)|\uparrow\rangle + \exp(\mathrm{i}\phi)\sin(\theta/2)|\downarrow\rangle$$



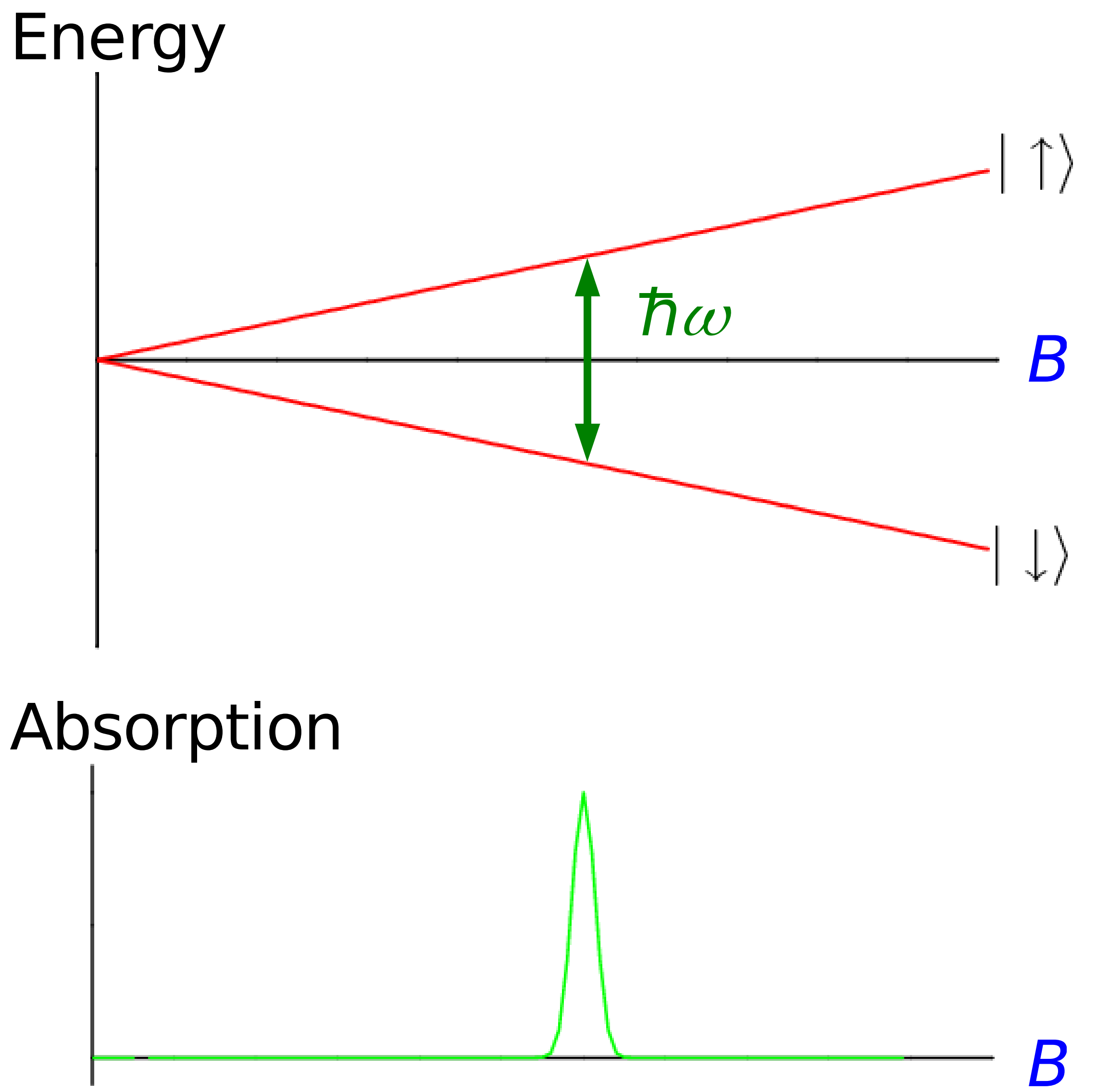
T_1: energy-changing (θ changes)
- spontaneous emission
- phonon coupling
- perturbations like σ_x, σ_y

T_2: phase-changing (ϕ changes)
- fluctuations in local magnetic field
- perturbations like σ_z

All T_1 processes are also T_2 processes

Continuous wave magnetic resonance

Apply radiation (B_1) and sweep field (B_0), measure absorption:



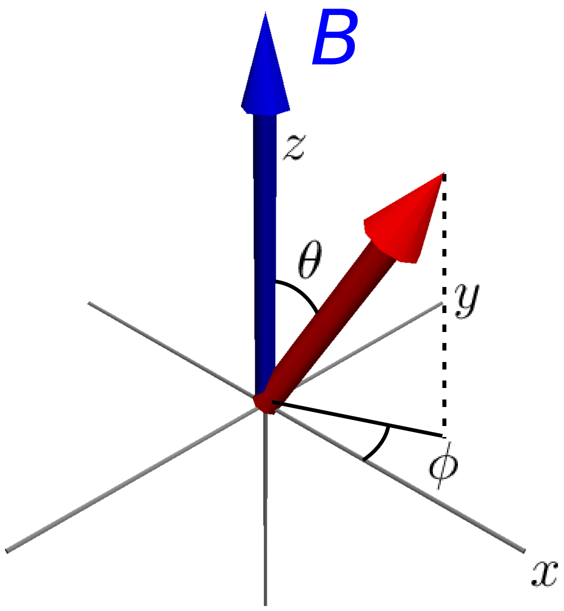
Continuous wave magnetic resonance requirements

Absorption occurs on resonance:

- $\omega = g\mu B$
- thermal polarization

- T_1 < Rabi period

Pulsed magnetic resonance



Apply static field (B_0)

Apply radiation (B_1) pulses

- duration determines θ change (θ-pulse)
- phase determines axis of rotation

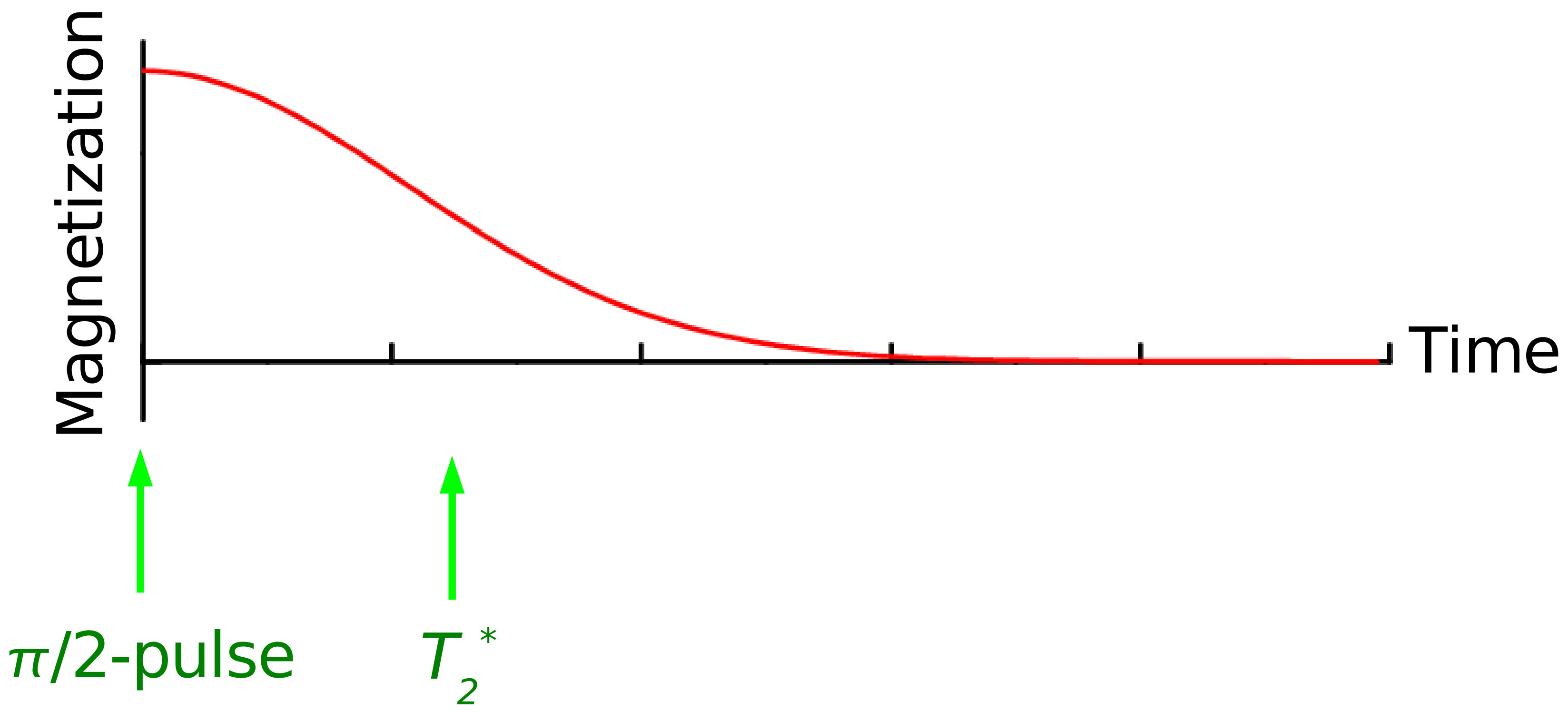
$$\mathcal{R}_\theta^\phi = \begin{pmatrix} \cos(\theta/2) & \mathrm{i}\exp(-\mathrm{i}\phi)\sin(\theta/2) \\ \exp(\mathrm{i}\phi)\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

Detect transient ensemble magnetization in rotating frame along x- and y- axes

Technical aspects of a pulsed magnetic resonance spectrometer

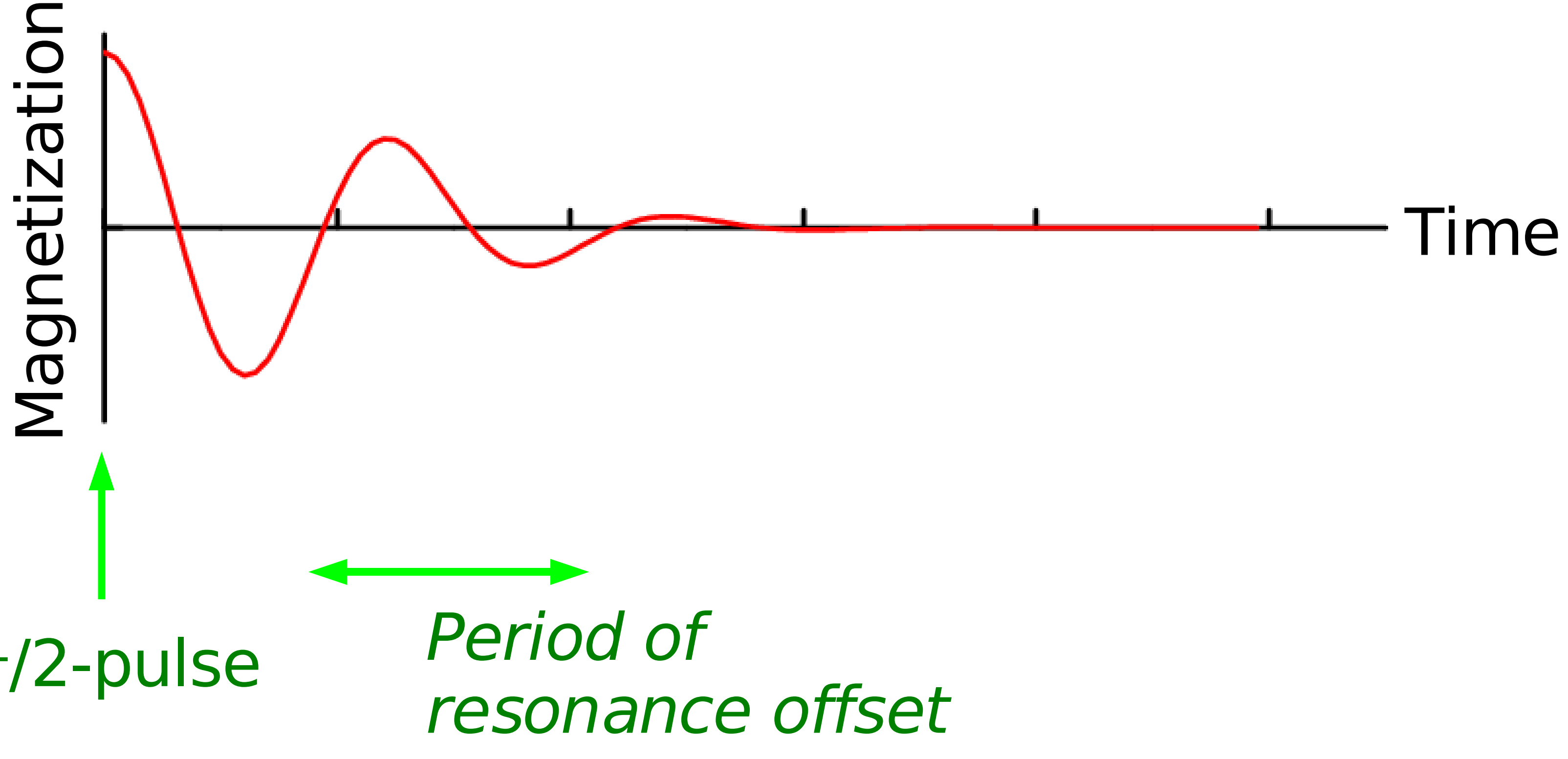
Free induction decay

Response to π/2-pulse on resonance:



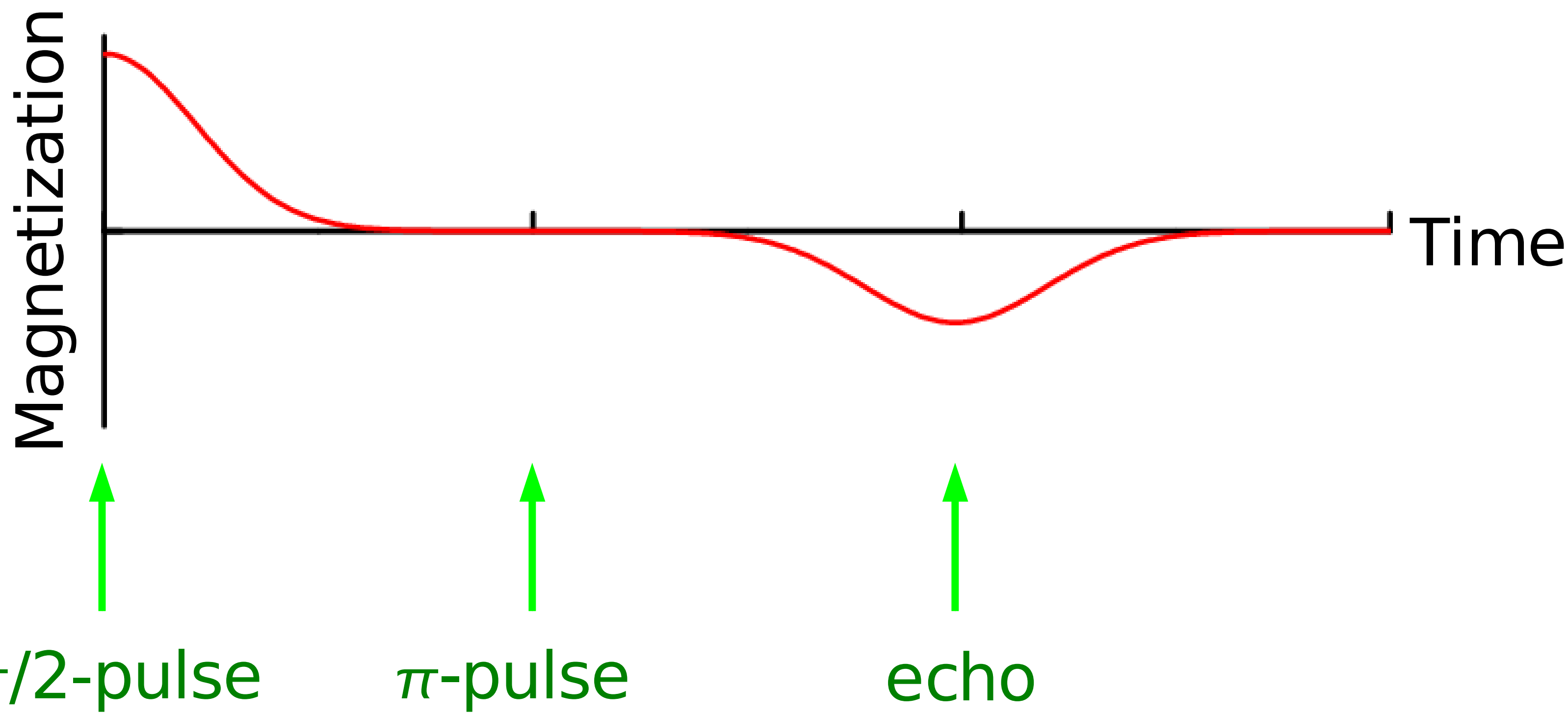
Free induction decay

Response to π/2-pulse off resonance:



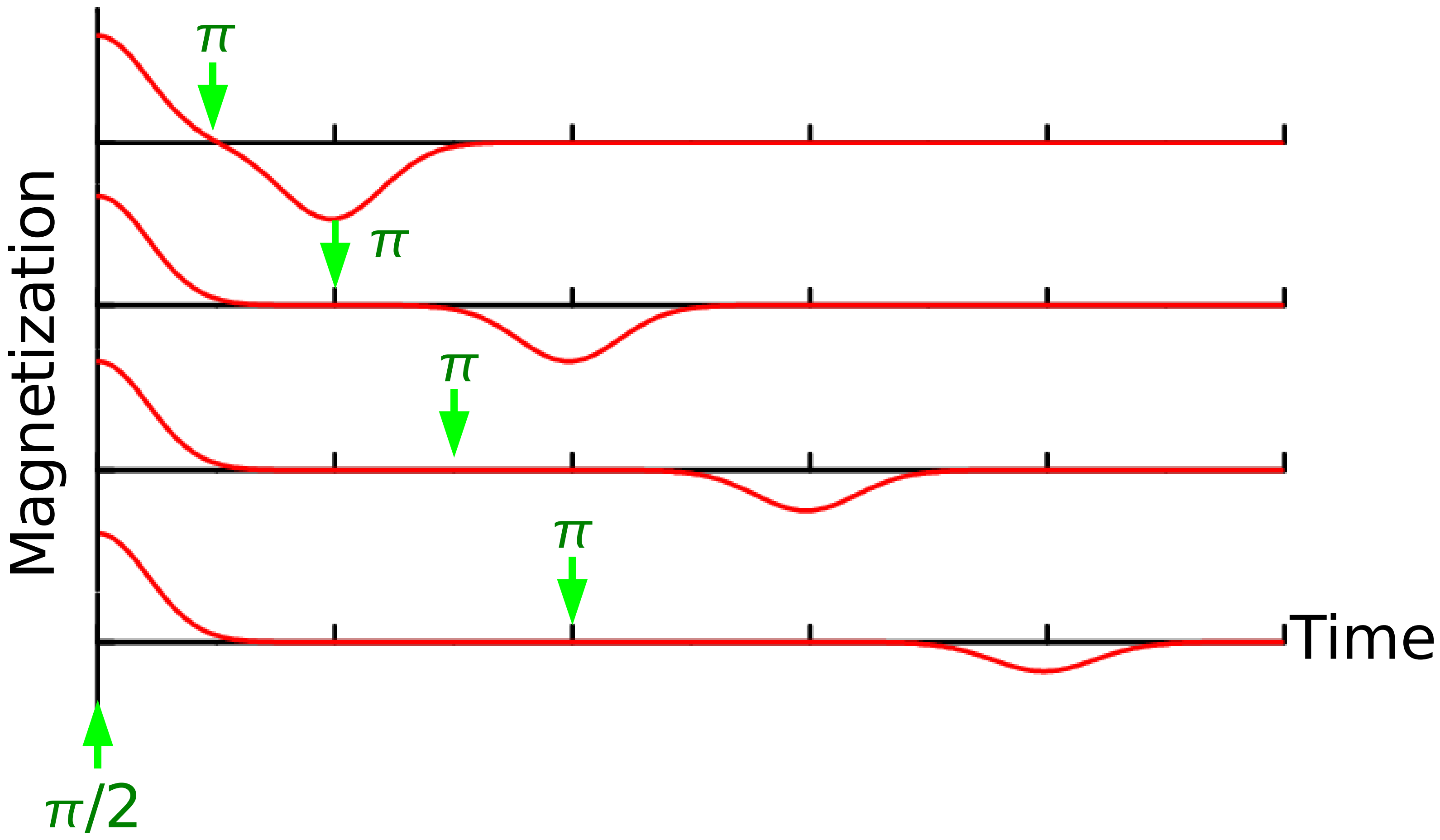
Hahn echo

Refocus dephasing with π-pulse:



Measuring T_2

Vary τ in $\pi/2 - \tau - \pi - \tau -$ echo:

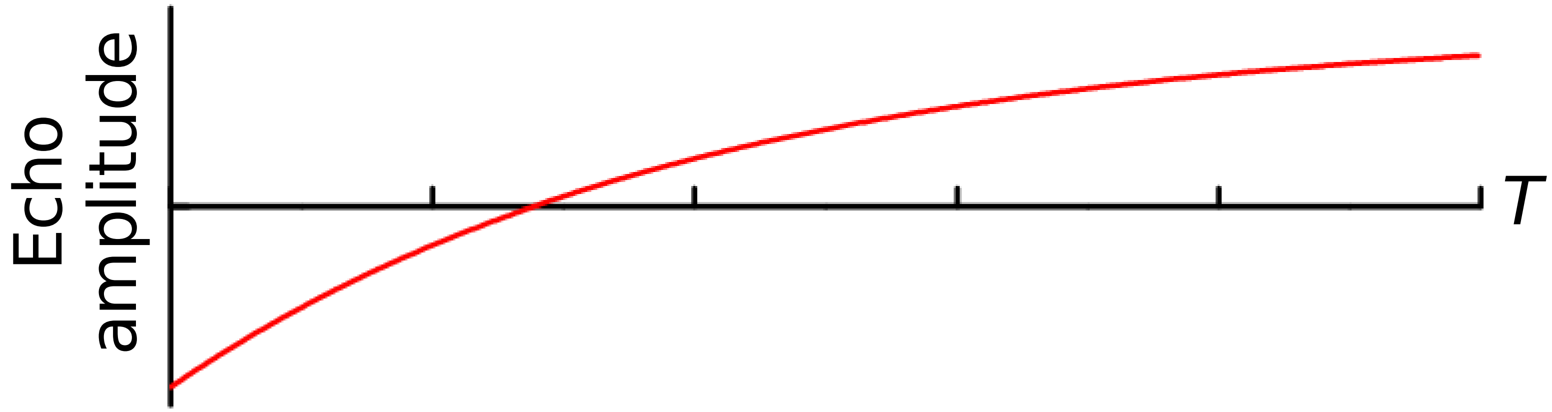


Measuring T_1

- FID or short Hahn echo sequence measures z-axis magnetization
- Inversion recovery sequence:

  $\pi - T - \pi/2 - \tau - \pi - \tau -$ echo

  with τ short and T varying

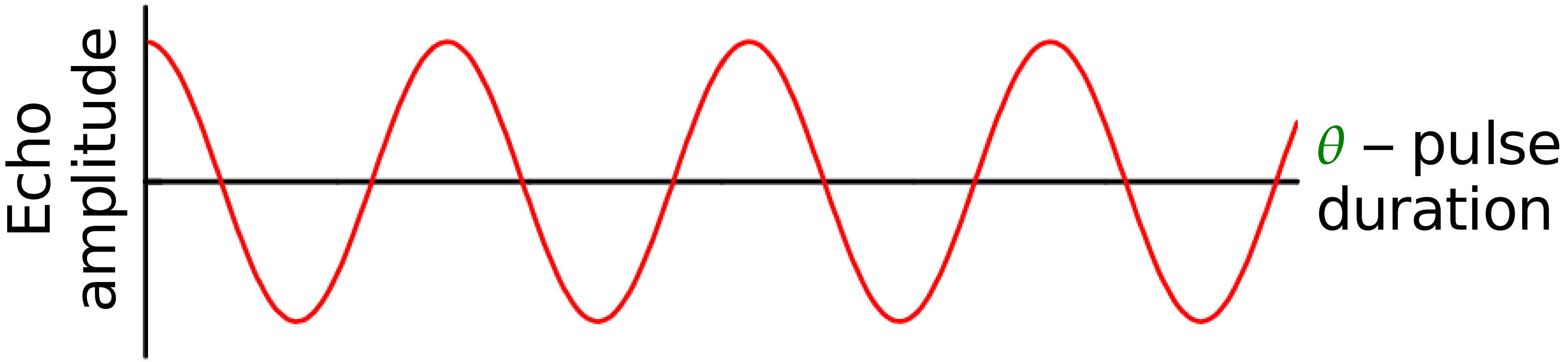


Rabi oscillations

- FID or short Hahn echo sequence measures *z*-axis magnetization
- Rabi oscillations:

  $\theta - T - \pi/2 - \tau - \pi - \tau -$ echo

  with T, τ both short



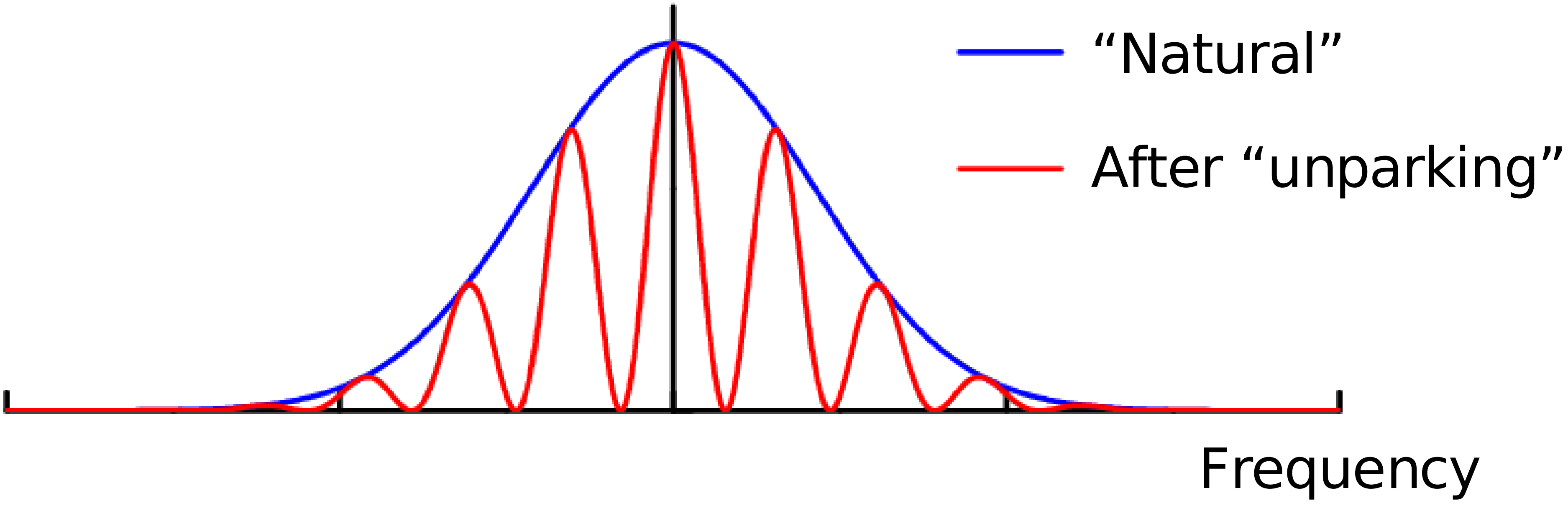
For completeness: stimulated echo

Breaking the refocussing pulse into two:

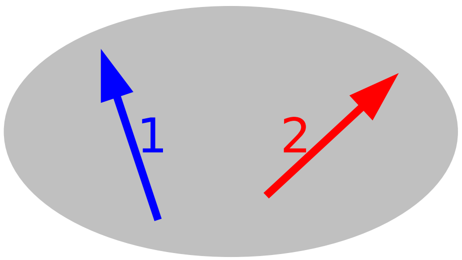
$\pi/2$ – τ – $\pi/2$ – T – $\pi/2$ – τ – echo

- T can be long ($T_2 < T < T_1$)

Spin packet distribution



Two qubits



$$\begin{aligned}\mathcal{H} &= \epsilon_1\sigma_z^1 + \epsilon_2\sigma_z^2 - J\sigma^1\cdot\sigma^2 \\ &= \epsilon_1\sigma_z^1 + \epsilon_2\sigma_z^2 - J\sigma_z^1\sigma_z^2 - J(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2)\end{aligned}$$

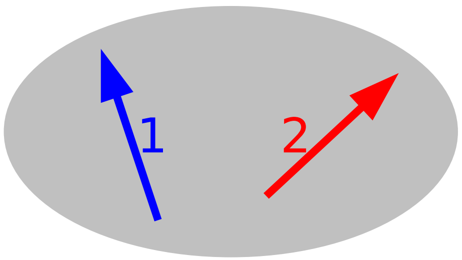
$$\begin{aligned}\sigma_+ &= \sigma_x + \mathrm{i}\sigma_y \\ \sigma_- &= \sigma_x - \mathrm{i}\sigma_y\end{aligned}$$

$$\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2 = \frac{1}{2}(\sigma_+^1\sigma_-^2 + \sigma_-^1\sigma_+^2)$$

To first order, for small *J*,

$$\mathcal{H} = \epsilon_1\sigma_z^1 + \epsilon_2\sigma_z^2 - J\sigma_z^1\sigma_z^2$$

Two qubits



$$\mathcal{H} = \epsilon_1 \sigma_z^1 + \epsilon_2 \sigma_z^2 - J \sigma_z^1 \sigma_z^2$$

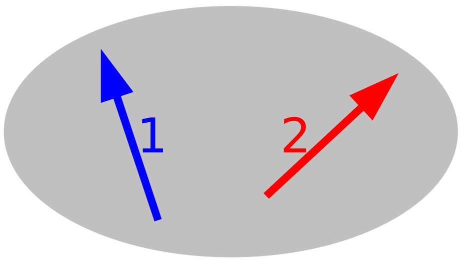
$\uparrow \uparrow$ —— $\epsilon_1 + \epsilon_2 - J$

$\uparrow \downarrow$ —— $\epsilon_1 - \epsilon_2 + J$

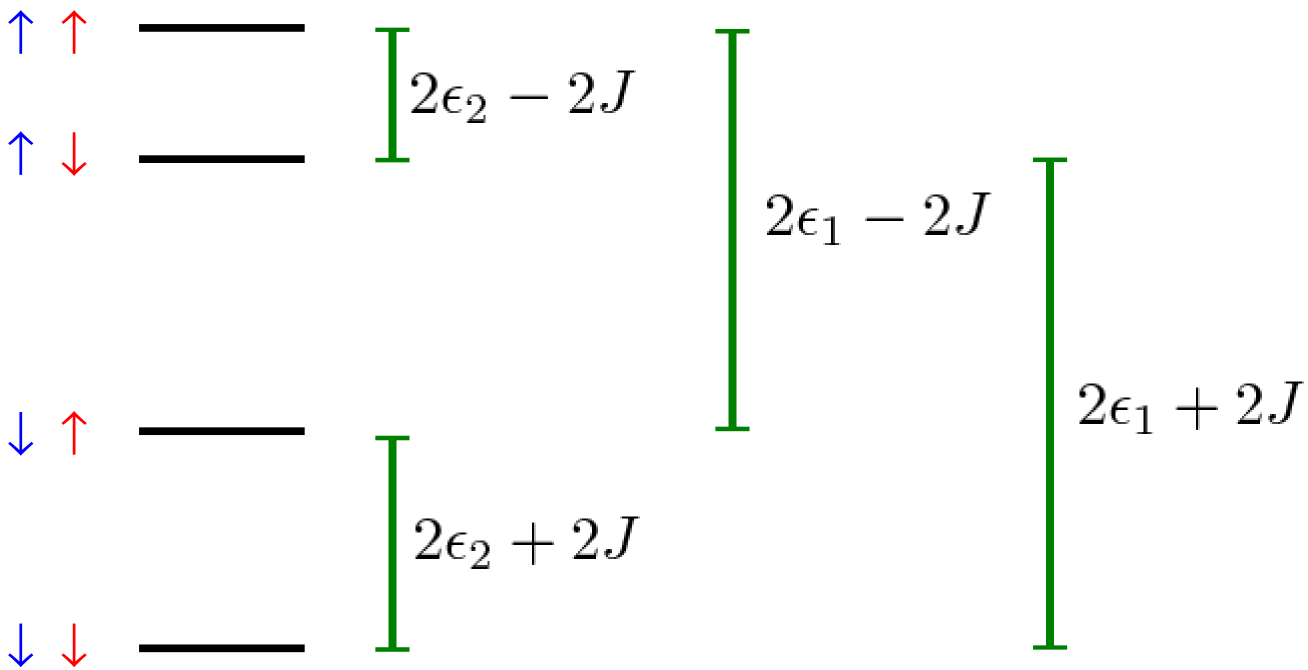
$\downarrow \uparrow$ —— $-\epsilon_1 + \epsilon_2 + J$

$\downarrow \downarrow$ —— $-\epsilon_1 - \epsilon_2 - J$

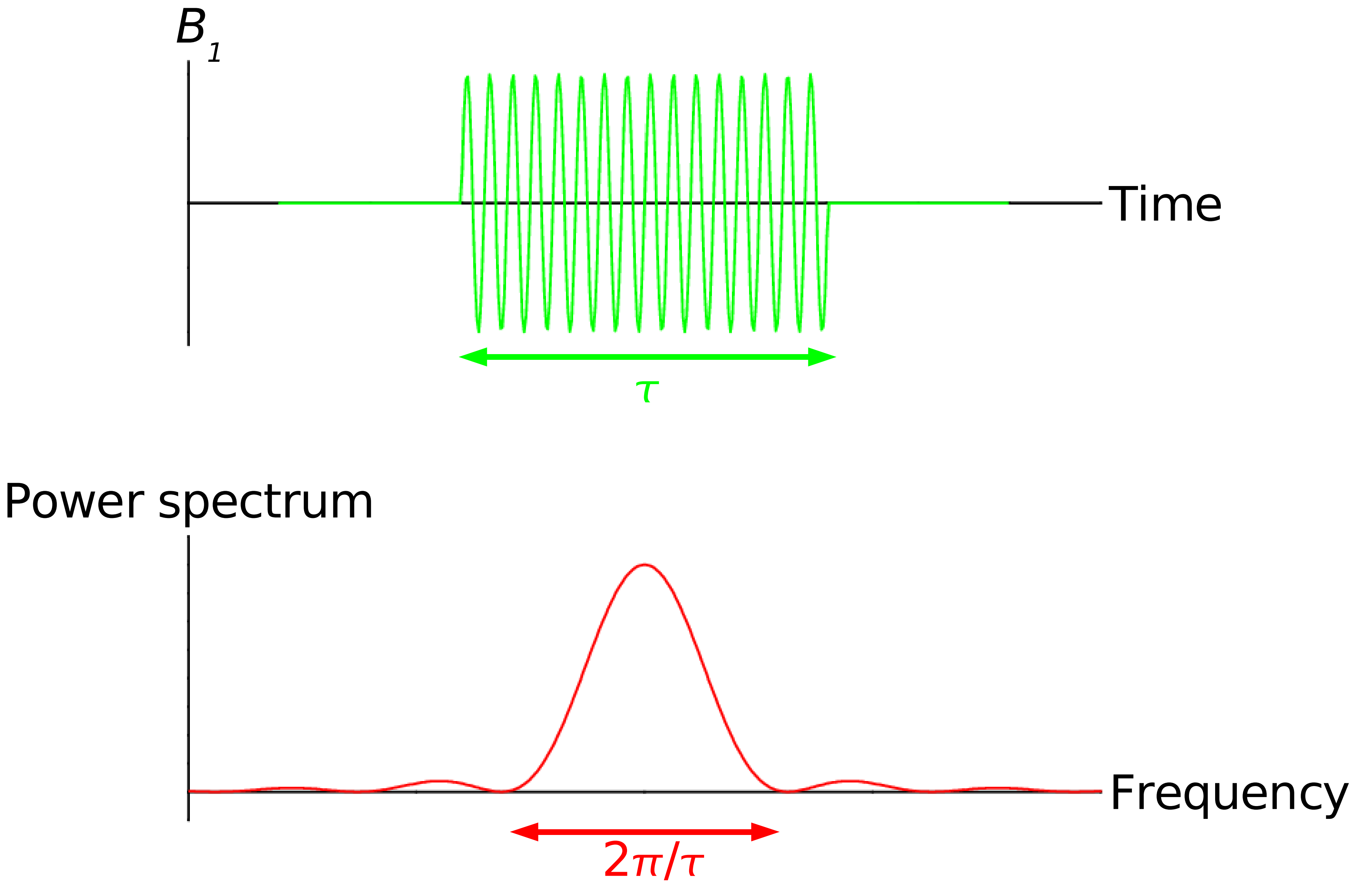
Two qubits: CNOT



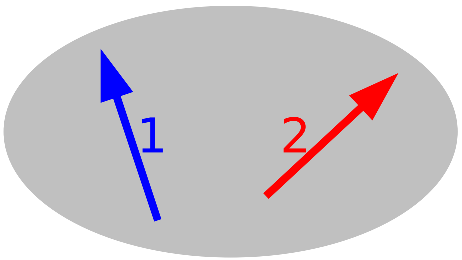
$$\mathcal{H} = \epsilon_1 \sigma_z^1 + \epsilon_2 \sigma_z^2 - J \sigma_z^1 \sigma_z^2$$



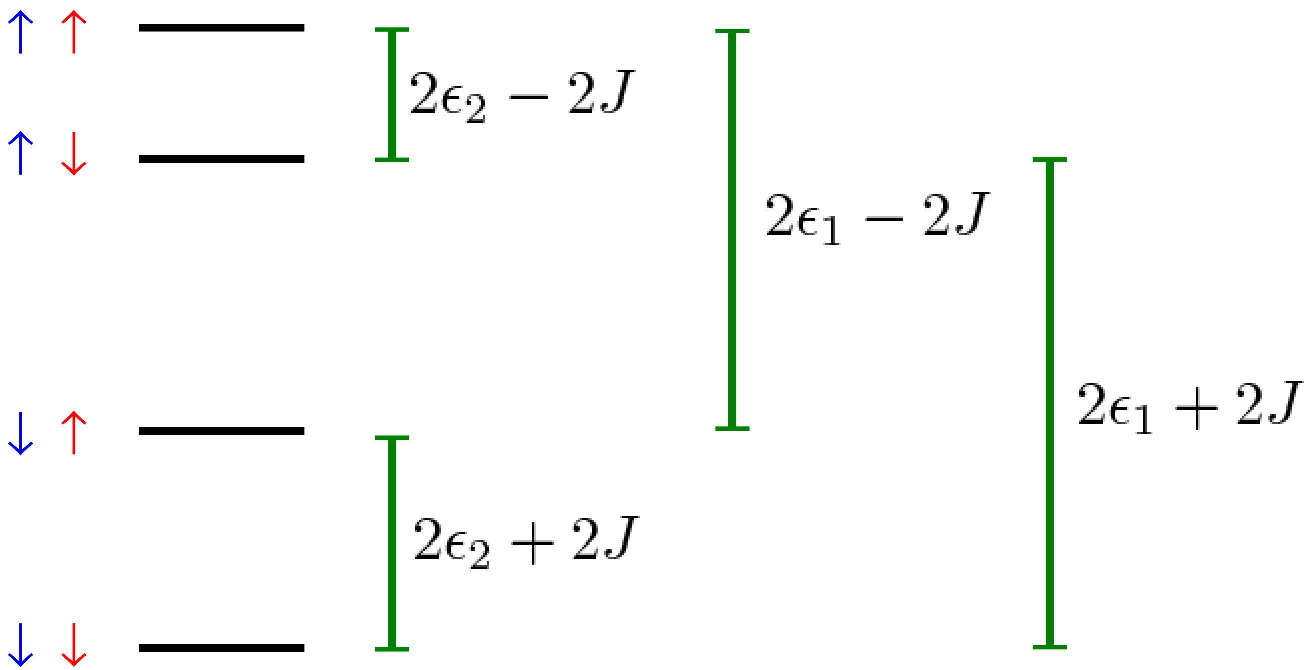
Bandwidths and selectivity



Two qubits: CNOT

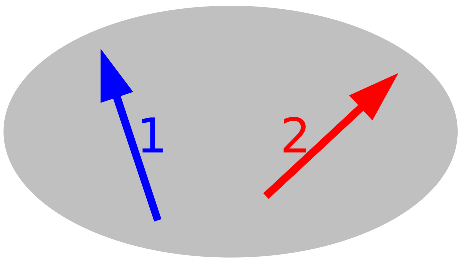


$$\mathcal{H} = \epsilon_1 \sigma_z^1 + \epsilon_2 \sigma_z^2 - J \sigma_z^1 \sigma_z^2$$

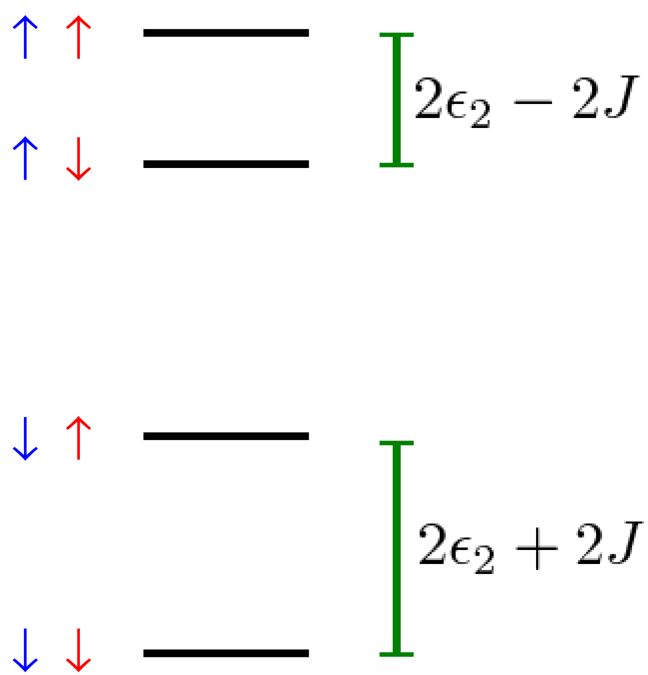


Selective pulses: $h/\tau \ll 4J$

Two qubits: unconditional NOT

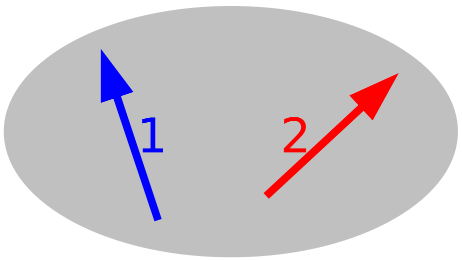


$$\mathcal{H} = \epsilon_1 \sigma_z^1 + \epsilon_2 \sigma_z^2 - J \sigma_z^1 \sigma_z^2$$

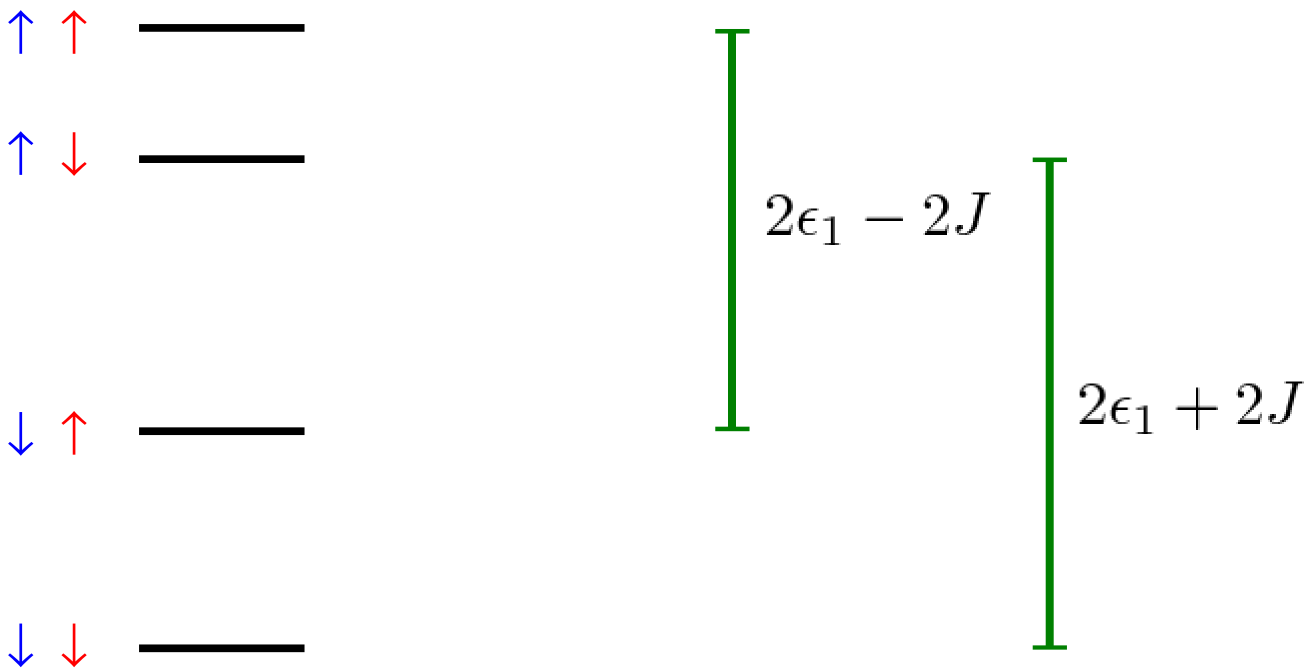


Non-selective pulses: $h/\tau \sim 4J$

Two qubits: unconditional NOT



$$\mathcal{H} = \epsilon_1 \sigma_z^1 + \epsilon_2 \sigma_z^2 - J \sigma_z^1 \sigma_z^2$$



Non-selective pulses: $h/\tau \sim 4J$

Nuclear magnetic resonance quantum computing

- Nuclear moments → qubits

  For protons, $\omega = 2\pi.42$ MHz/Tesla,
  Zeeman splittings ~ 1 to 10 μeV

- NMR → single-qubit unitary transformations

- "Through-bond" coupling → multiqubit gates

  J ~ 10 to 100 Hz

- Spin-echo / free induction decay from ensemble → readout

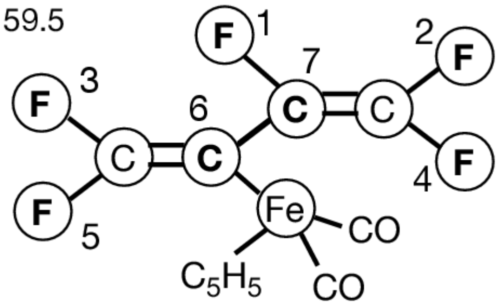
Nuclear magnetic resonance quantum computing

Experimental realization of Shor's quantum factoring algorithm using nuclear magnetic resonance

Lieven M. K. Vandersypen*†, Matthias Steffen*†, Gregory Breyta*, Costantino S. Yannoni*, Mark H. Sherwood* & Isaac L. Chuang*†

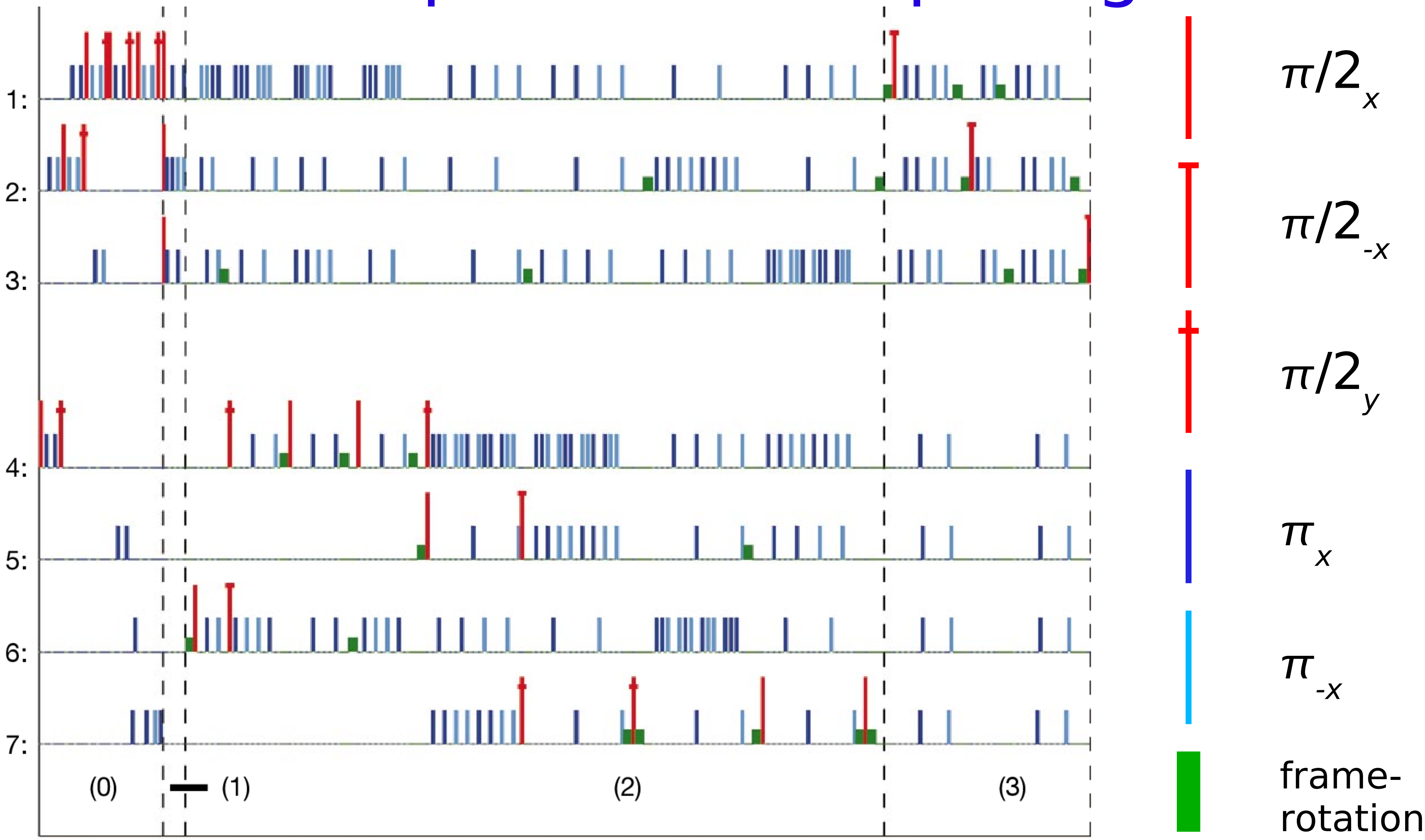
** IBM Almaden Research Center, San Jose, California 95120, USA*
† Solid State and Photonics Laboratory, Stanford University, Stanford, California 94305-4075, USA

i	$\omega_i/2\pi$	$T_{1,i}$	$T_{2,i}$	J_{7i}	J_{6i}	J_{5i}	J_{4i}	J_{3i}	J_{2i}
1	–22052.0	5.0	1.3	–221.0	37.7	6.6	–114.3	14.5	25.16
2	489.5	13.7	1.8	18.6	–3.9	2.5	79.9	3.9	
3	25088.3	3.0	2.5	1.0	–13.5	41.6	12.9		
4	–4918.7	10.0	1.7	54.1	–5.7	2.1			
5	15186.6	2.8	1.8	19.4	59.5				
6	–4519.1	45.4	2.0	68.9					
7	4244.3	31.6	2.0						



Vandersypen et al., Nature **414** 883 (2001)

Nuclear magnetic resonance quantum computing



Vandersypen et al., Nature **414** 883 (2001)

The problem with NMR computers

- For protons, $\omega = 2\pi.42$ MHz/Tesla,
  Zeeman splittings ~ 1 to 10 μeV ~ 10 to 100 mK
- Experiments performed at room temperature
- Members of ensemble start in different states!

Density operator

- Each member in state $|\psi_i\rangle$ with probability p_i
- Define $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$
- Properties:
  - $\mathrm{Tr}\ \rho = 1$
  - $\mathrm{Tr}\ \rho\hat{A} = \langle\hat{A}\rangle$

E.g.

$$\mathrm{Tr}\ \rho\sigma_z = \mathrm{Tr}\left[\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] = \langle\sigma_z\rangle$$

Density operator

- Each member in state $|\psi_i\rangle$ with probability p_i
- Define $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$
- Properties:
  - $\mathrm{Tr}\ \rho = 1$
  - $\mathrm{Tr}\ \rho\hat{A} = \langle\hat{A}\rangle$

E.g.

$$\mathrm{Tr}\ \rho\sigma_x = \mathrm{Tr}\left[\begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = \langle\sigma_x\rangle$$

Density operator

- Each member in state $|\psi_i\rangle$ with probability p_i
- Define $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$
- Properties:
  - $\mathrm{Tr}\ \rho = 1$
  - $\mathrm{Tr}\ \rho\hat{A} = \langle\hat{A}\rangle$
  - Under the action of *U*, $\rho \xrightarrow{U} U\rho U^\dagger$

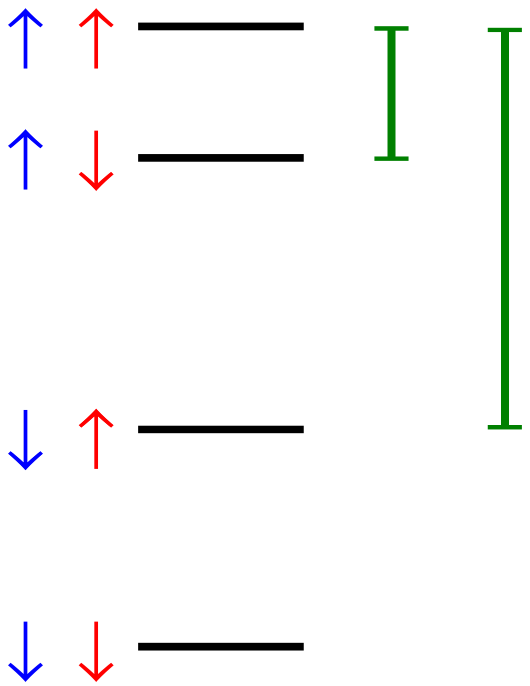
The "pseudo-pure" state

Thermal density matrix:

$$\rho_{\mathrm{th}} = \begin{pmatrix} p_0 & 0 & 0 & \cdots & \\ 0 & p_1 & 0 & \cdots & \\ 0 & 0 & p_2 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \\ & & & & p_{m-1} \end{pmatrix}, \quad p_i = \frac{\exp(-E_i/k_B T)}{\sum_i \exp(-E_i/k_B T)}$$

Pure state: $$\rho_{\mathrm{pure}} = \begin{pmatrix} 1 & 0 & 0 & \cdots & \\ 0 & 0 & 0 & \cdots & \\ 0 & 0 & 0 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \\ & & & & 0 \end{pmatrix}$$

The “pseudo-pure” state



Incoherent illumination “saturates” transition

- equalizes populations

The “pseudo-pure” state

Thermal density matrix:

$$\rho_{\mathrm{th}} = \begin{pmatrix} p_0 & 0 & 0 & \cdots & \\ 0 & p_1 & 0 & \cdots & \\ 0 & 0 & p_2 & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \\ & & & & p_{m-1} \end{pmatrix}, \quad p_i = \frac{\exp(-E_i/k_BT)}{\sum_i \exp(-E_i/k_BT)}$$

Pseudo-pure state:

$$\begin{aligned} \rho_{\mathrm{pp}} &= \begin{pmatrix} p_0 & 0 & 0 & \cdots & \\ 0 & \bar{p} & 0 & \cdots & \\ 0 & 0 & \bar{p} & \cdots & \\ \vdots & \vdots & \vdots & \ddots & \\ & & & & \bar{p} \end{pmatrix}, \quad \bar{p} = \frac{1-p_0}{m-1} \\ &= (p_0 - \bar{p})\rho_{\mathrm{pure}} + \bar{p}\mathbf{I} \end{aligned}$$

The "pseudo-pure" state amplitude

Amplitude of pure part is $$p_0 - \bar{p} = p_0 - \frac{1-p_0}{m-1} = \frac{mp_0 - 1}{m-1}$$

$$\frac{E_i}{k_B T} \ll 1$$ and $$p_i = \frac{\exp(-E_i/k_B T)}{\sum_i \exp(-E_i/k_B T)}$$

$$p_0 \approx \frac{1+\delta}{m}$$ where $$\delta = -\frac{E_0}{k_B T}$$

$$p_0 - \bar{p} \approx \frac{\delta}{m-1} = \frac{\delta}{2^N - 1}$$

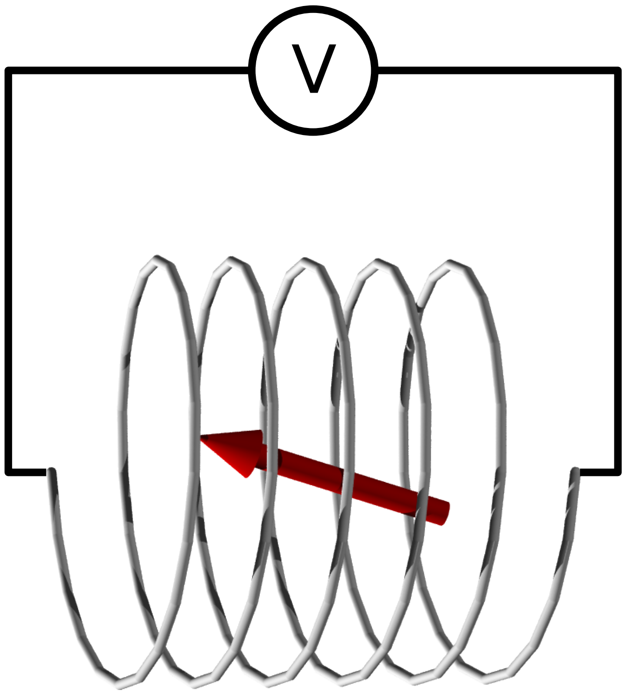
Nuclear magnetic resonance quantum computing

- Nuclear moments → qubits
- NMR → single-qubit unitary transformations
- "Through-bond" coupling → multiqubit gates
- Spin-echo / free induction decay from ensemble → readout
- Signal decays exponentially with computer size

For electrons, $\omega = 2\pi.28$ GHz/Tesla,
Zeeman splittings ~ 1 to 10 meV ~ 1 to 10 K

"Detection" vs. "Measurement"

Magnetic resonance detection apparatus:



Quantum mechanical measurement:

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \xrightarrow{\text{Measure } \sigma_z} \begin{cases} |\uparrow\rangle & p = |\alpha|^2 \\ |\downarrow\rangle & p = |\beta|^2 \end{cases}$$

Summary

- Pulsed magnetic resonance provides spin-based qubit manipulation techniques
  - single qubit gates
  - multi-qubit gates

- There are fundamental problems with scaling up to useful devices
  - pseudo-pure state
  - ensemble measurement