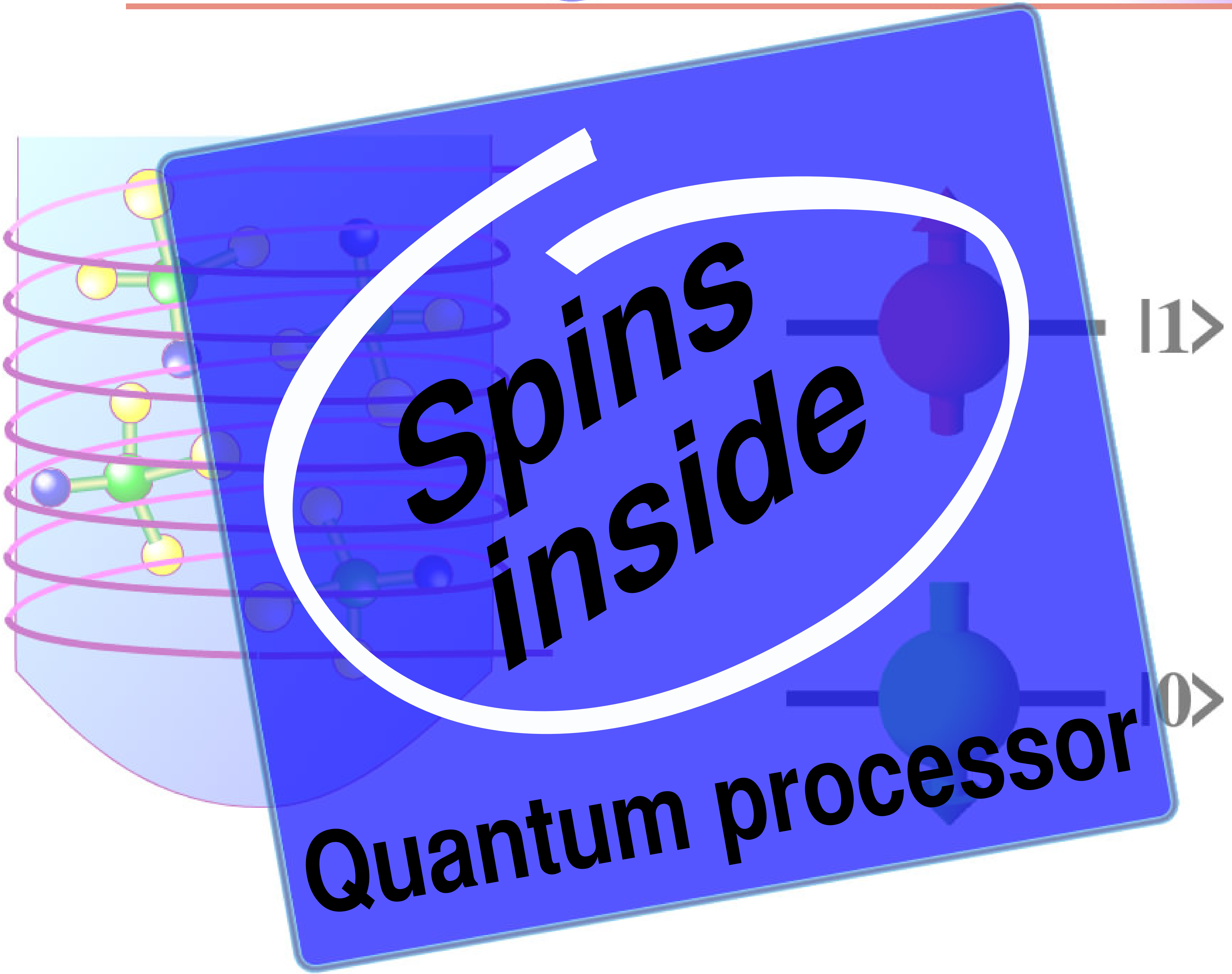
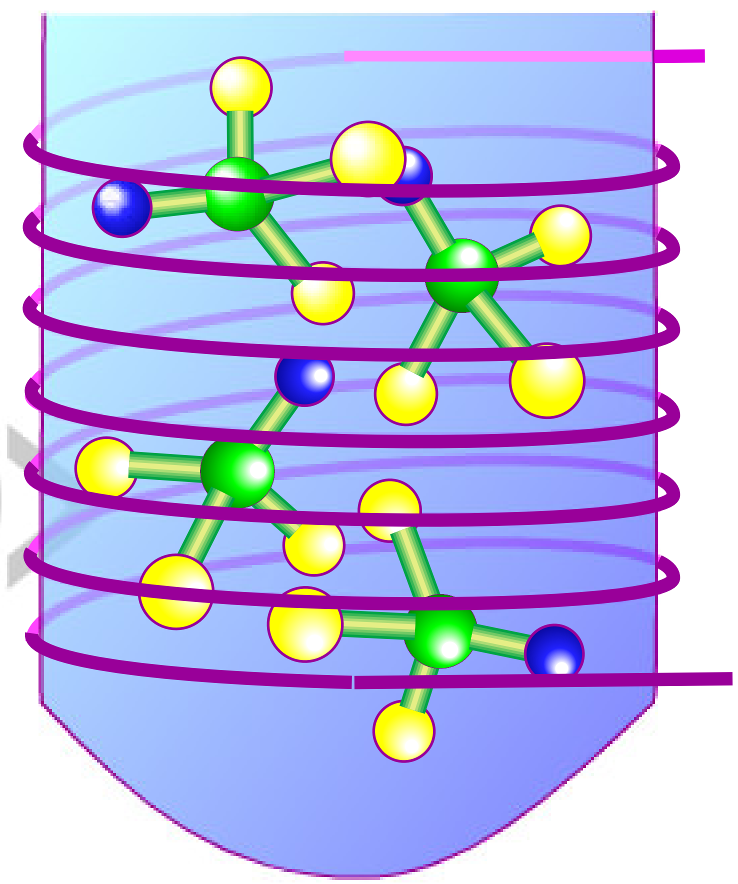
Nuclear Magnetic Resonance



Why Spins ?

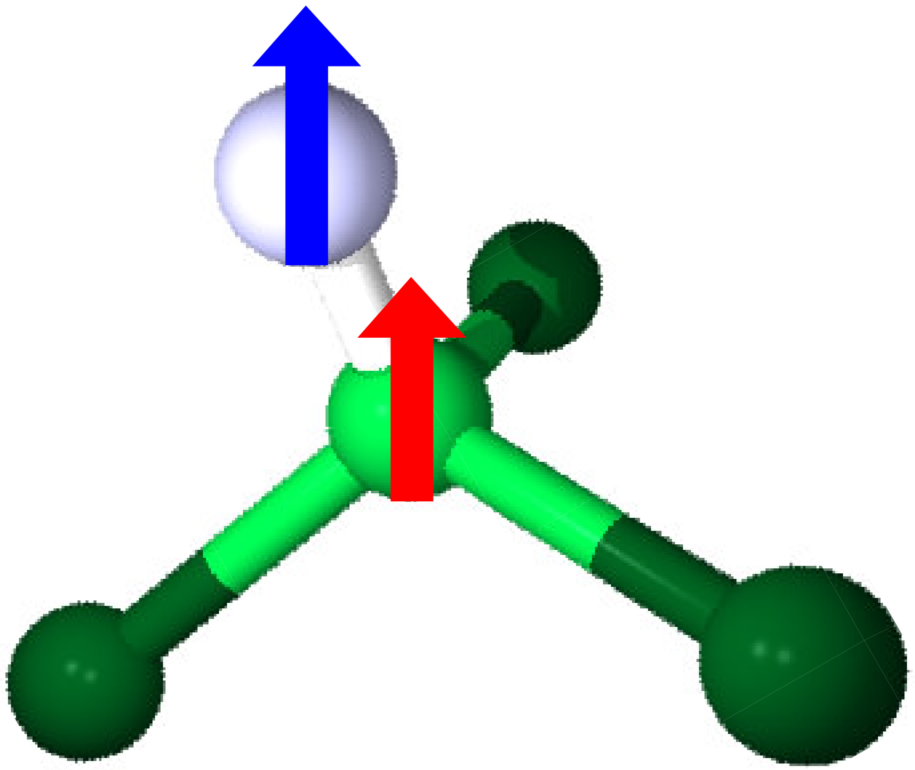
- Simple, well isolated quantum system
- Long decoherence times (~sec)
- Gate operations are "easy" to implement

\+ it works !



Ensemble QC

Qubits



Single spin detection difficult

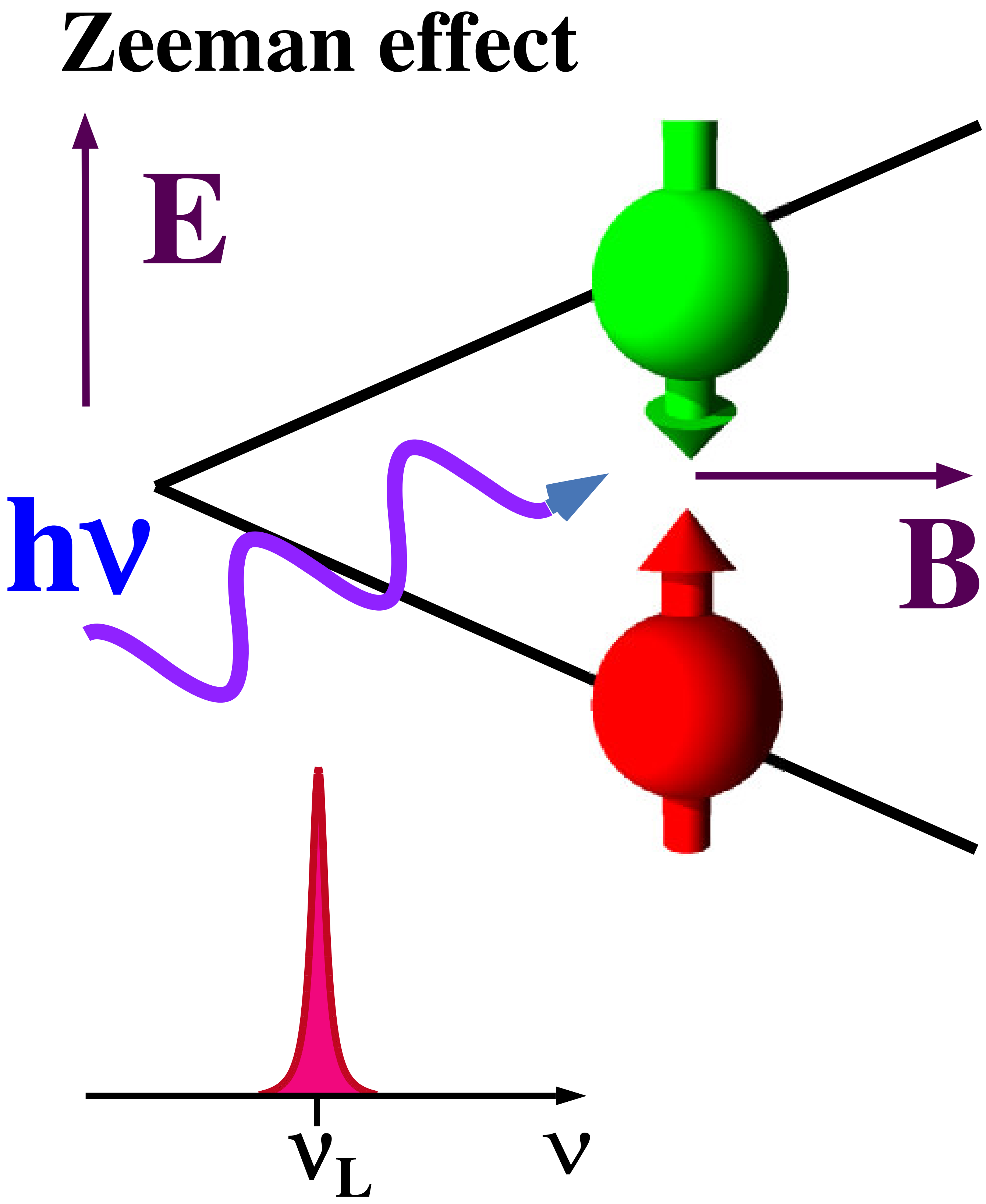
↓

use 10^{20} identical copies

↓

"Ensemble Quantum Computing"

Magnetic Resonance

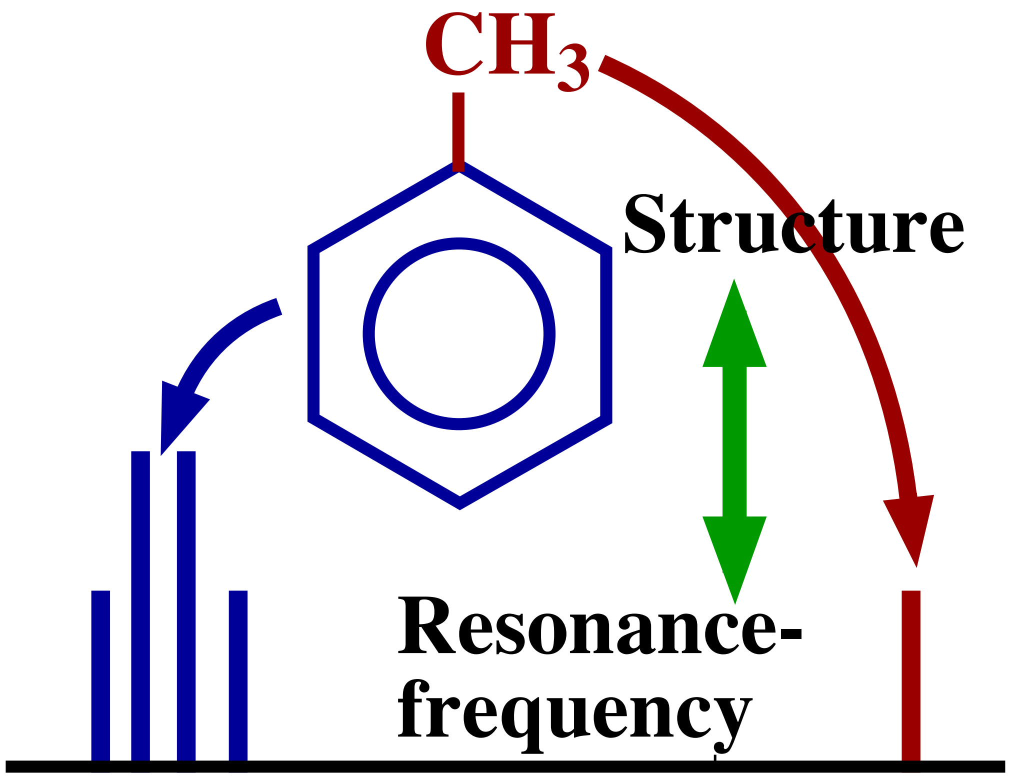


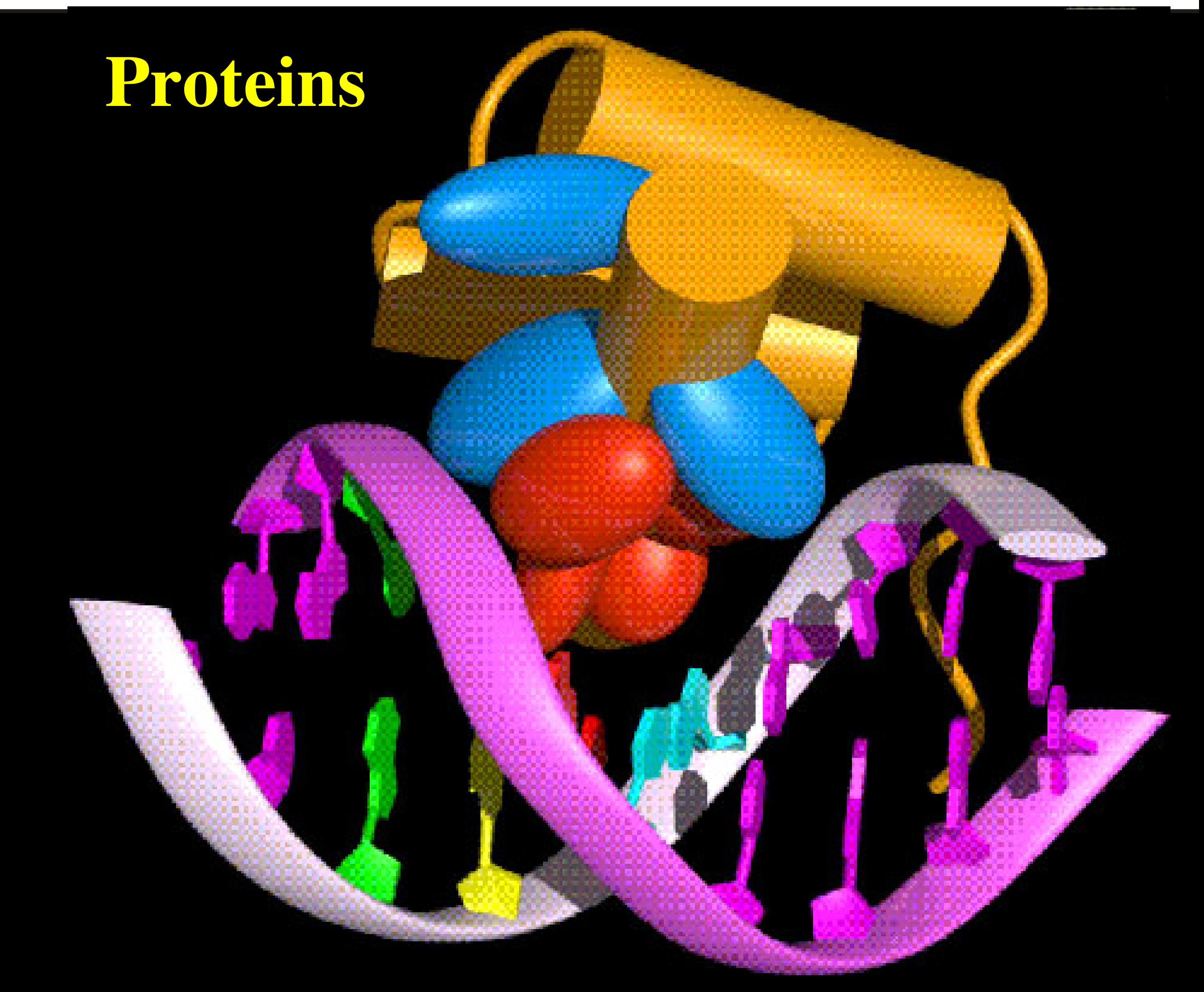
$$H_z = -\hbar\,\gamma\,\vec{B}\cdot\vec{I}$$
$$= -\hbar\,\gamma\,B_0\,I_z$$

Principle

MR measures tran-sitions between spin states, which are excited by a radio-frequency field.

Applications

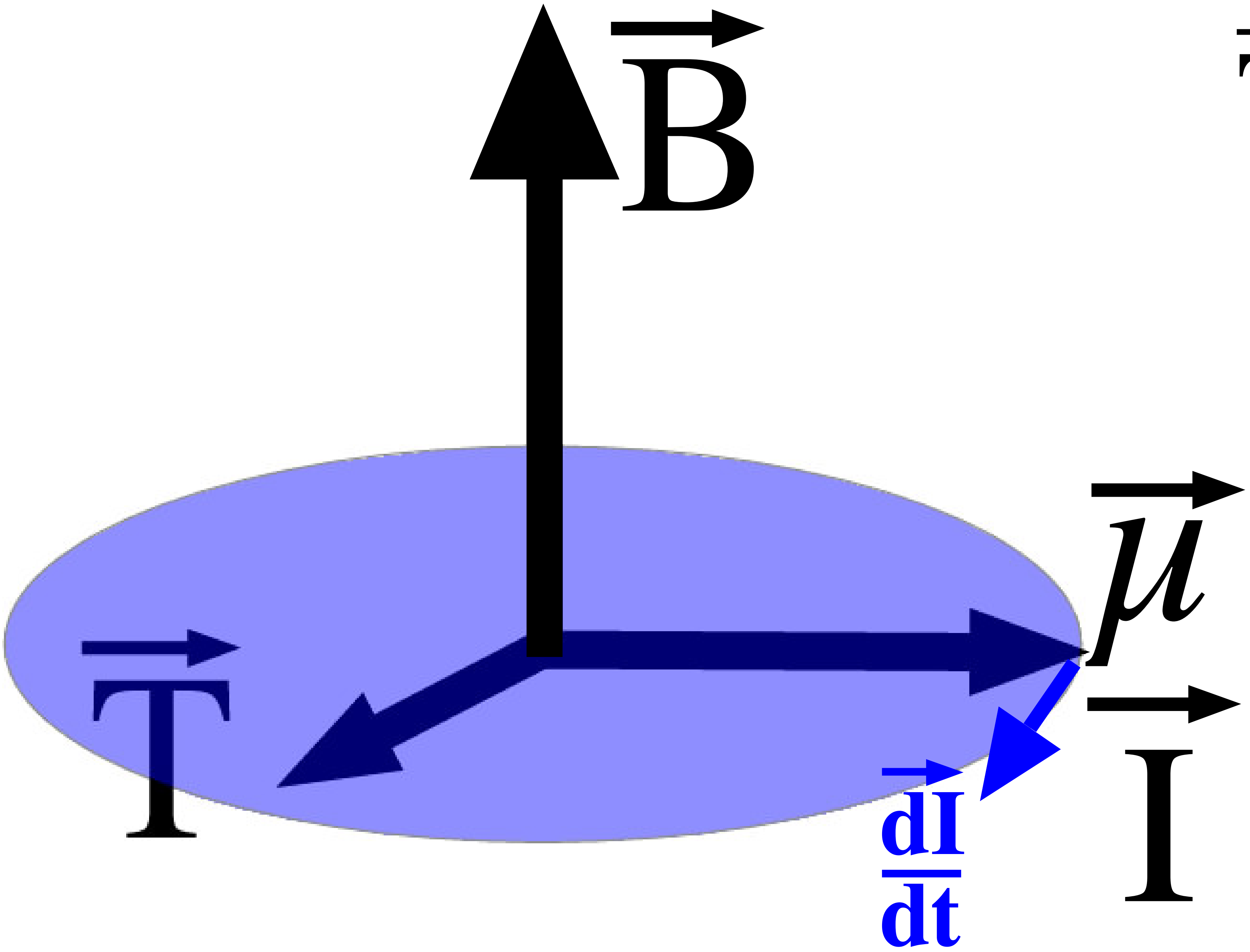




Magnetic Resonance Imaging


NMR Lab
600 MHz Solid State NMR
OXFORD

Equation of Motion



$$\vec{T} = \vec{\mu} \times \vec{B}$$
$$= -\gamma \vec{B} \times \vec{I}$$

Larmor Precession

Equation of motion:

$$\frac{dI_x}{dt} = -\omega_L I_y$$

$$\frac{dI_y}{dt} = \omega_L I_x$$

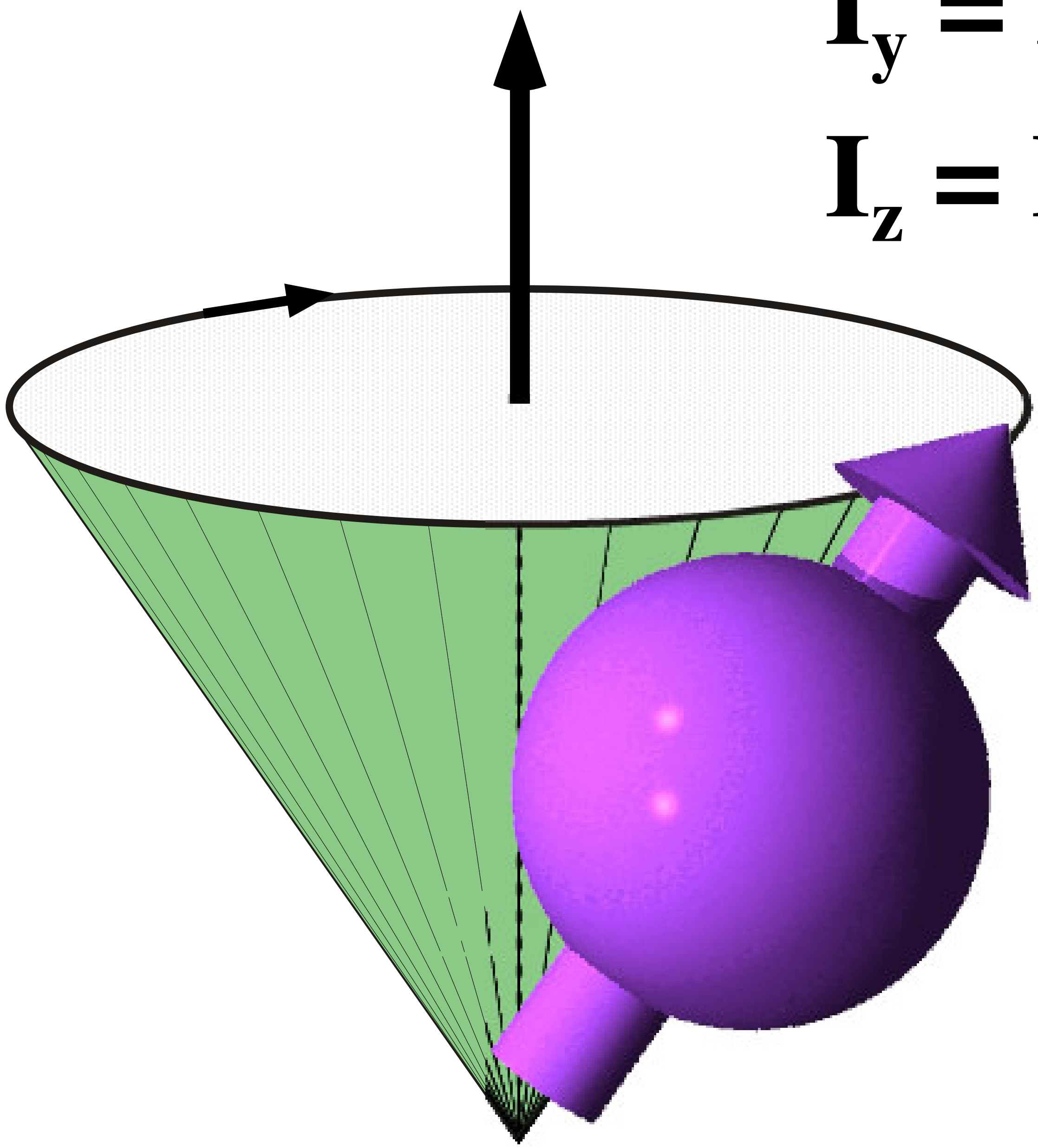
$$\frac{dI_z}{dt} = 0$$

Solution:

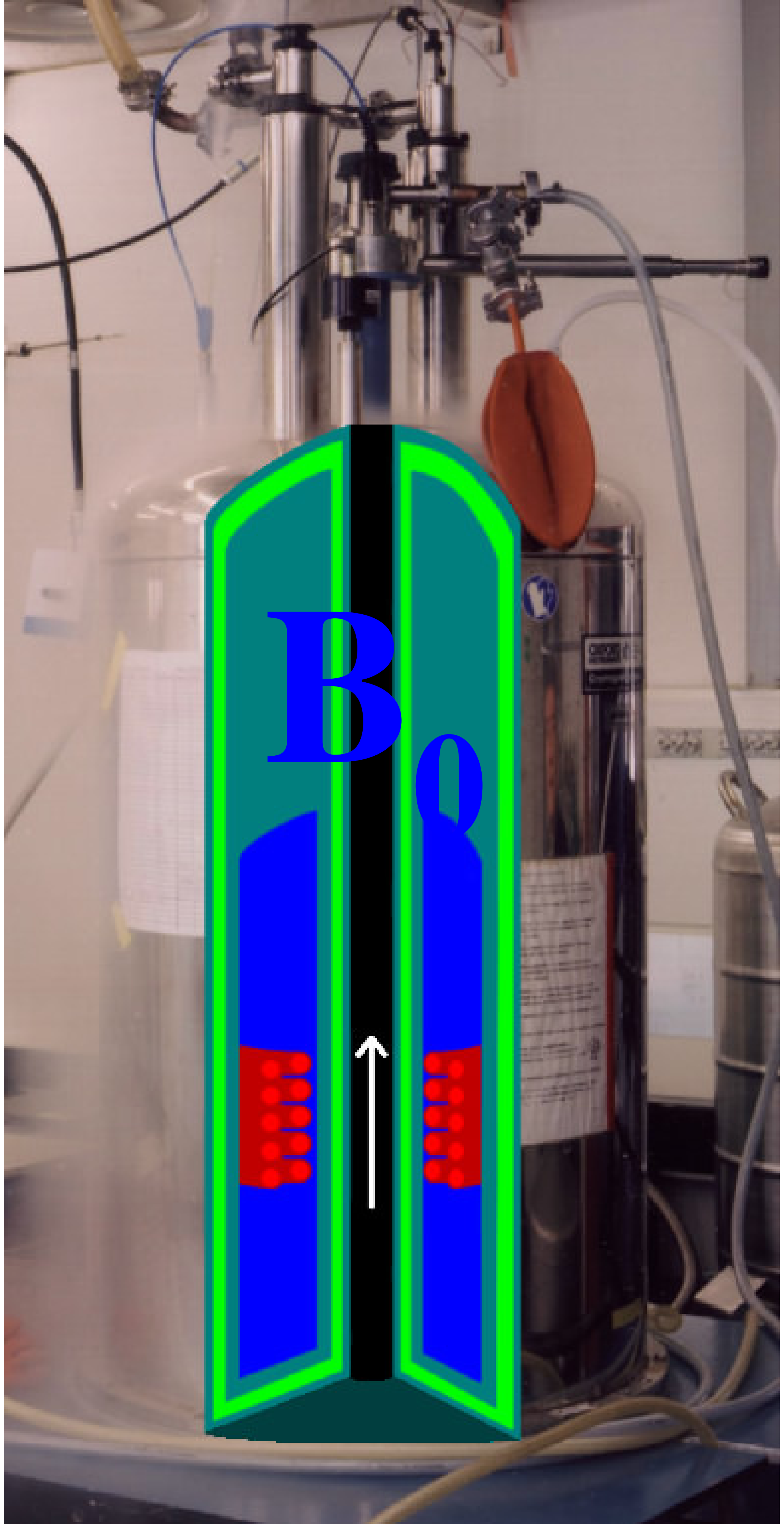
$$I_x = I_{xy} \cos(\omega_L t - \phi)$$

$$I_y = I_{xy} \sin(\omega_L t - \phi)$$

$$I_z = I_z(0)$$

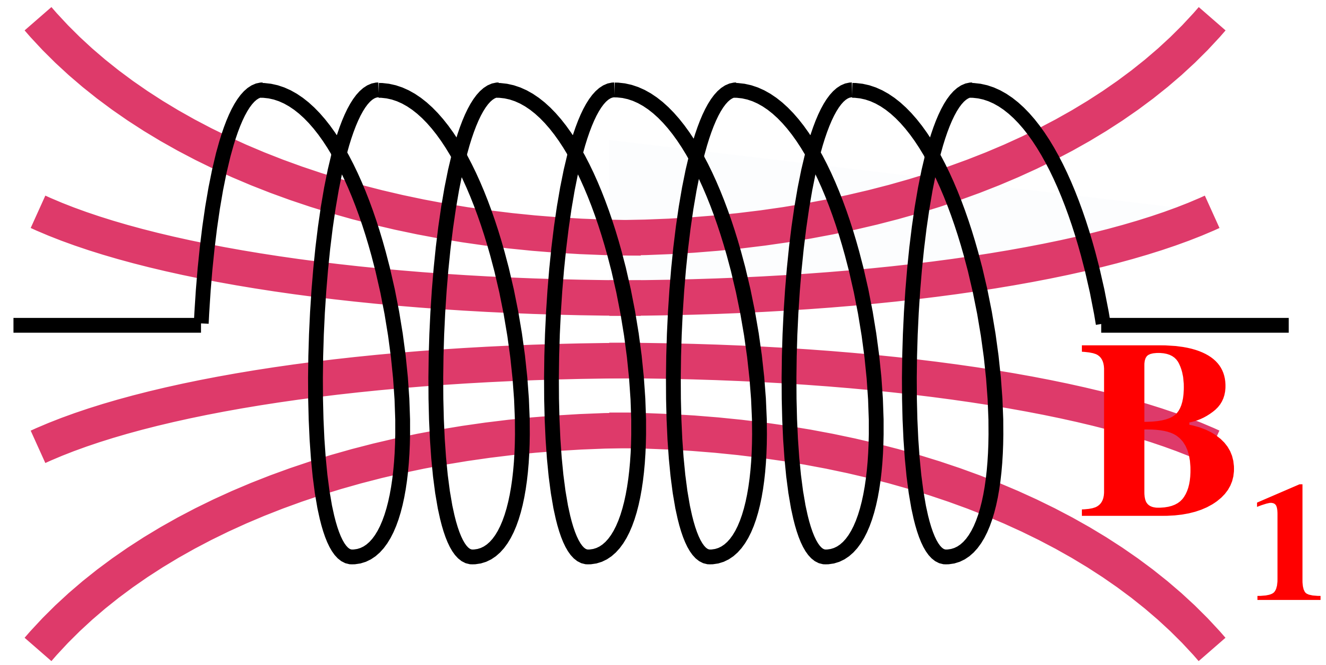


Excitation



magnetic radiofrequency field B_1

$\perp$ static magnetic field B_0



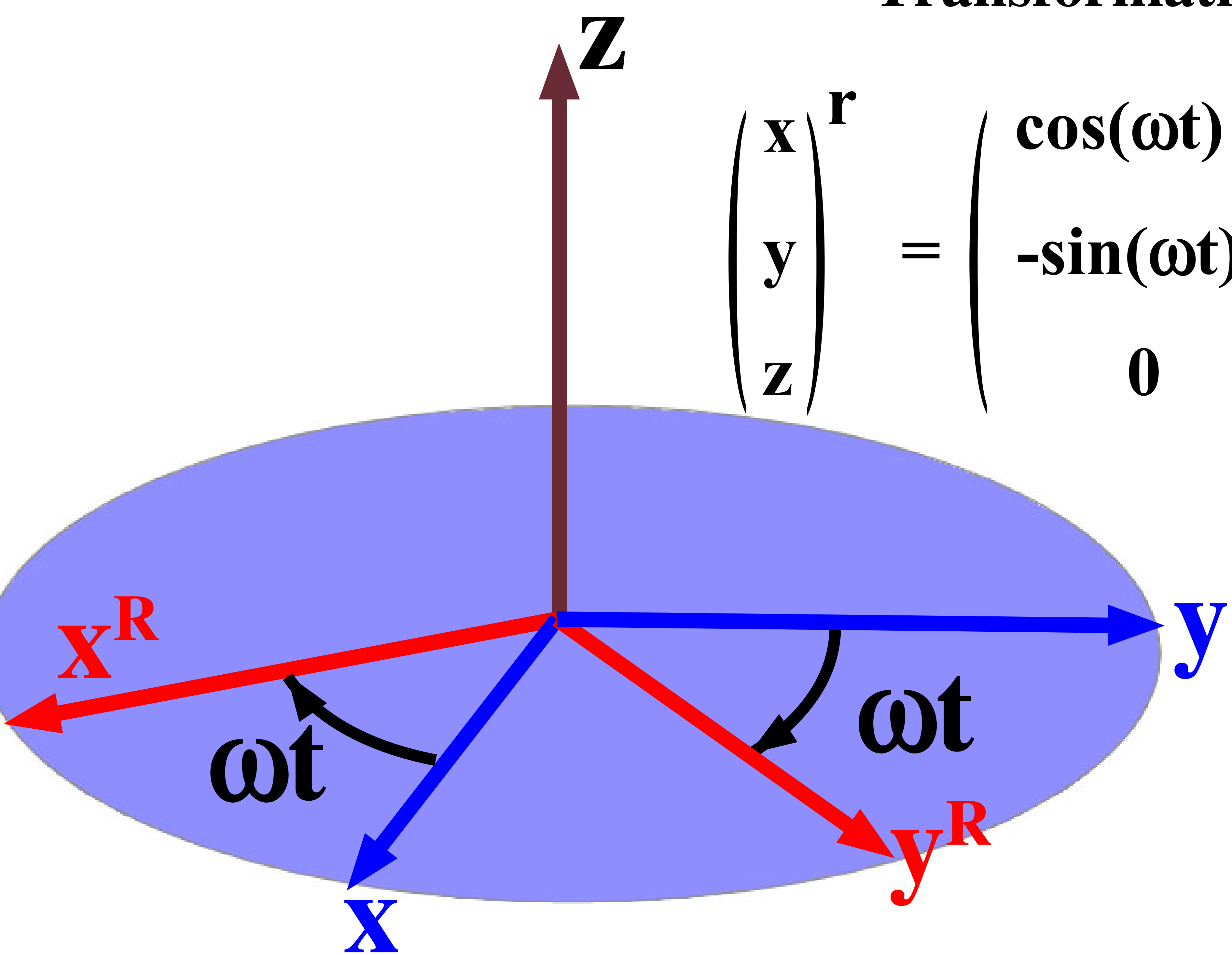
$$B_{rf} = 2\,B_1 \cos(\omega_{rf} t) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$= B_1 \begin{pmatrix} \cos(\omega_{rf} t) \\ \sin(\omega_{rf} t) \\ 0 \end{pmatrix} + B_1 \begin{pmatrix} \cos(\omega_{rf} t) \\ -\sin(\omega_{rf} t) \\ 0 \end{pmatrix}$$

Coordinate Systems

Transformation:

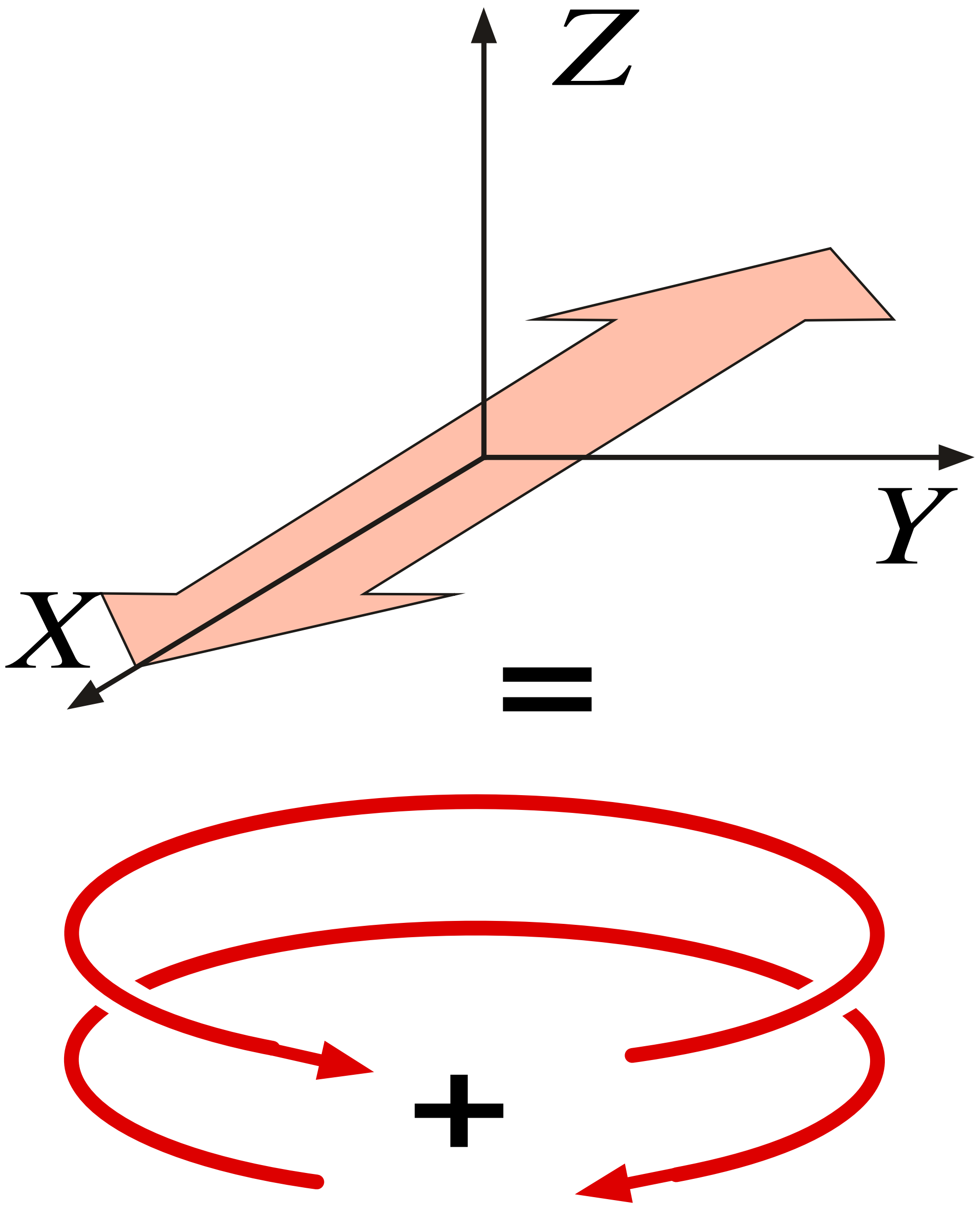
$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}^r = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) & 0 \\ -\sin(\omega t) & \cos(\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



Rotating Coordinate System

A) Lab Frame

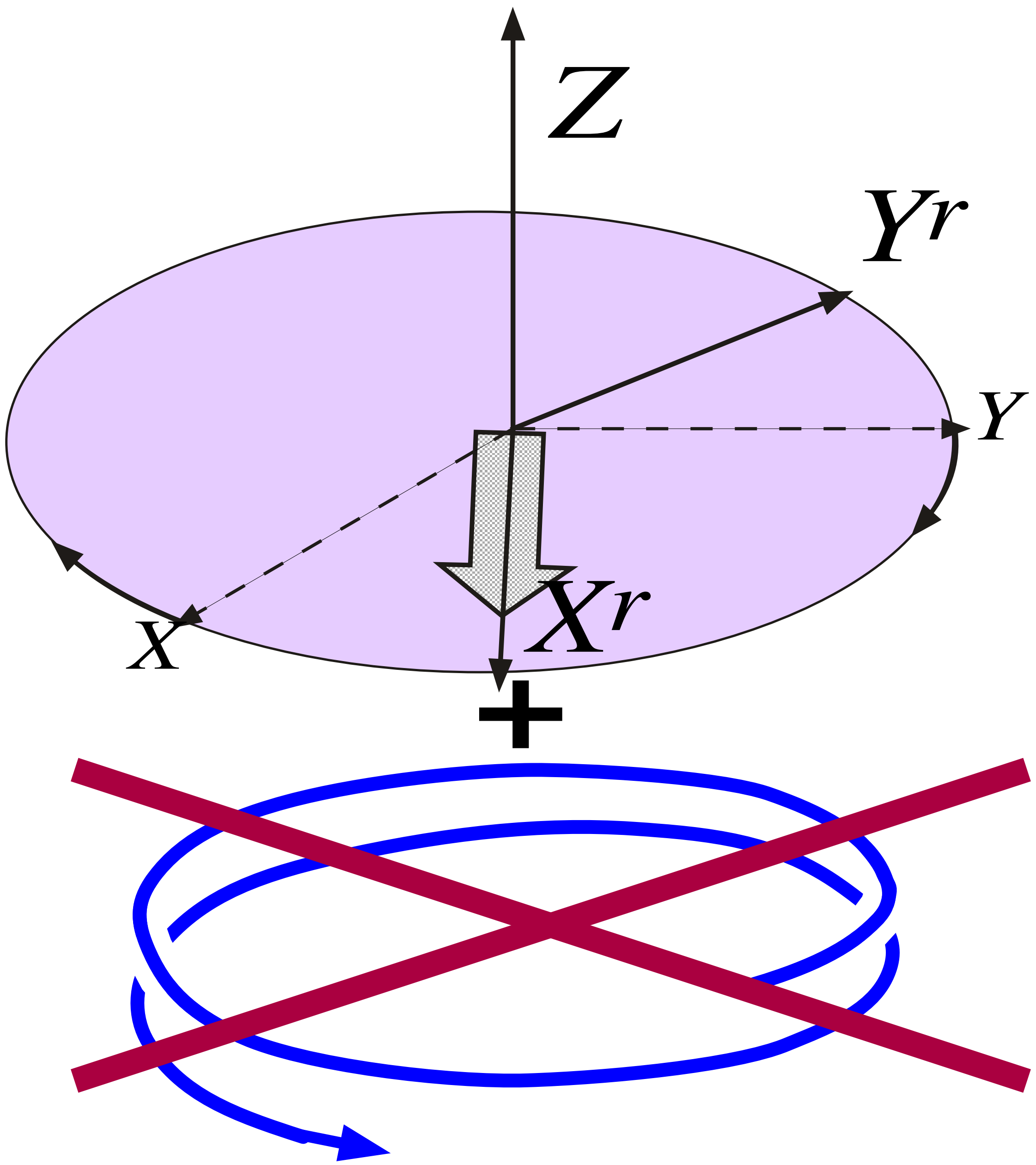
$(B_1, 0, 0)\ 2\cos(\omega_{rf}t)$



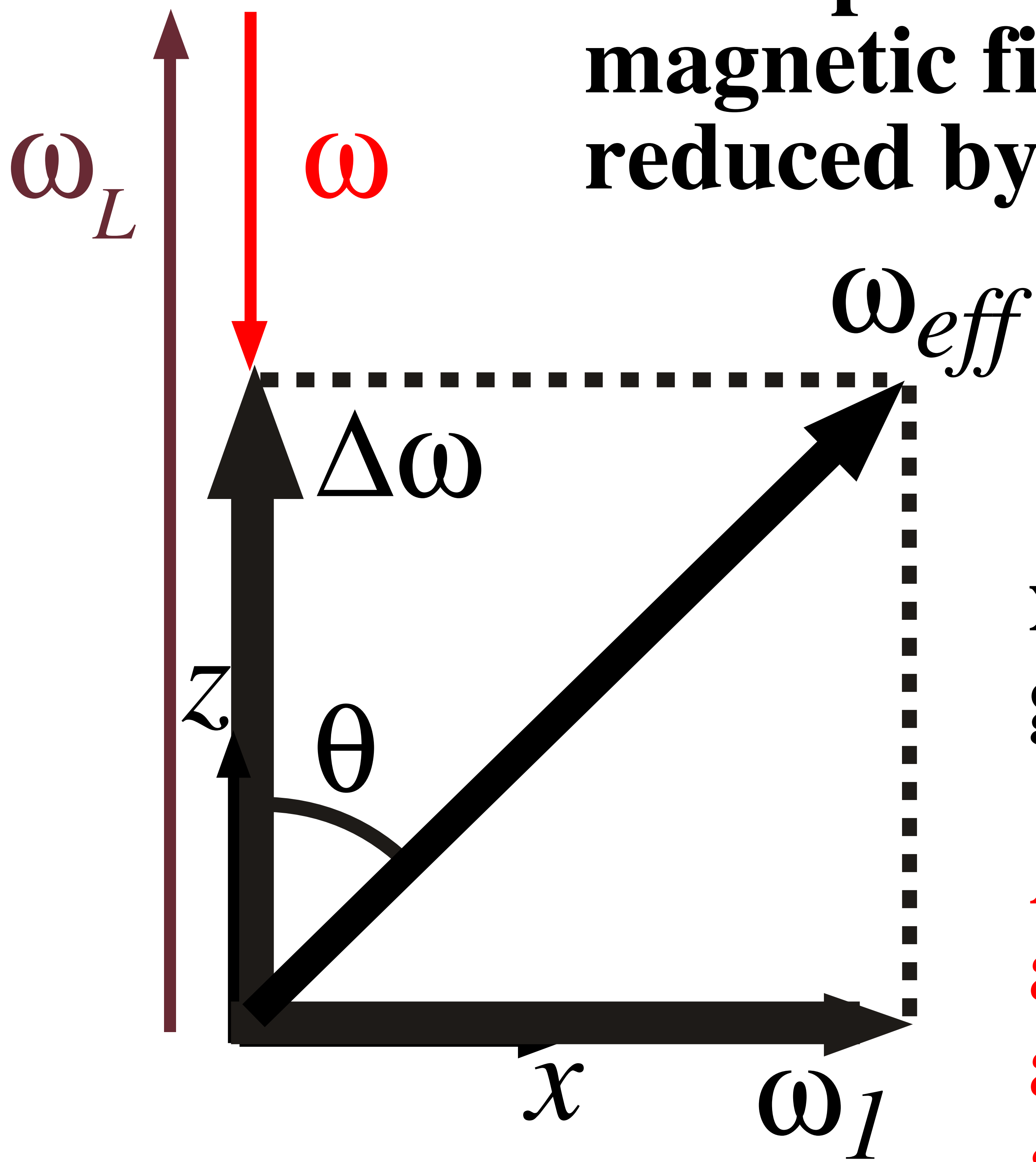
B) Rotating Frame

$(B_1, 0, 0)\ [1 + \cos(2\omega_{rf}t)]$

$-\ (0, B_1, 0)\ \sin(2\omega_{rf}t)$ neglect nonresonant



Effective Field



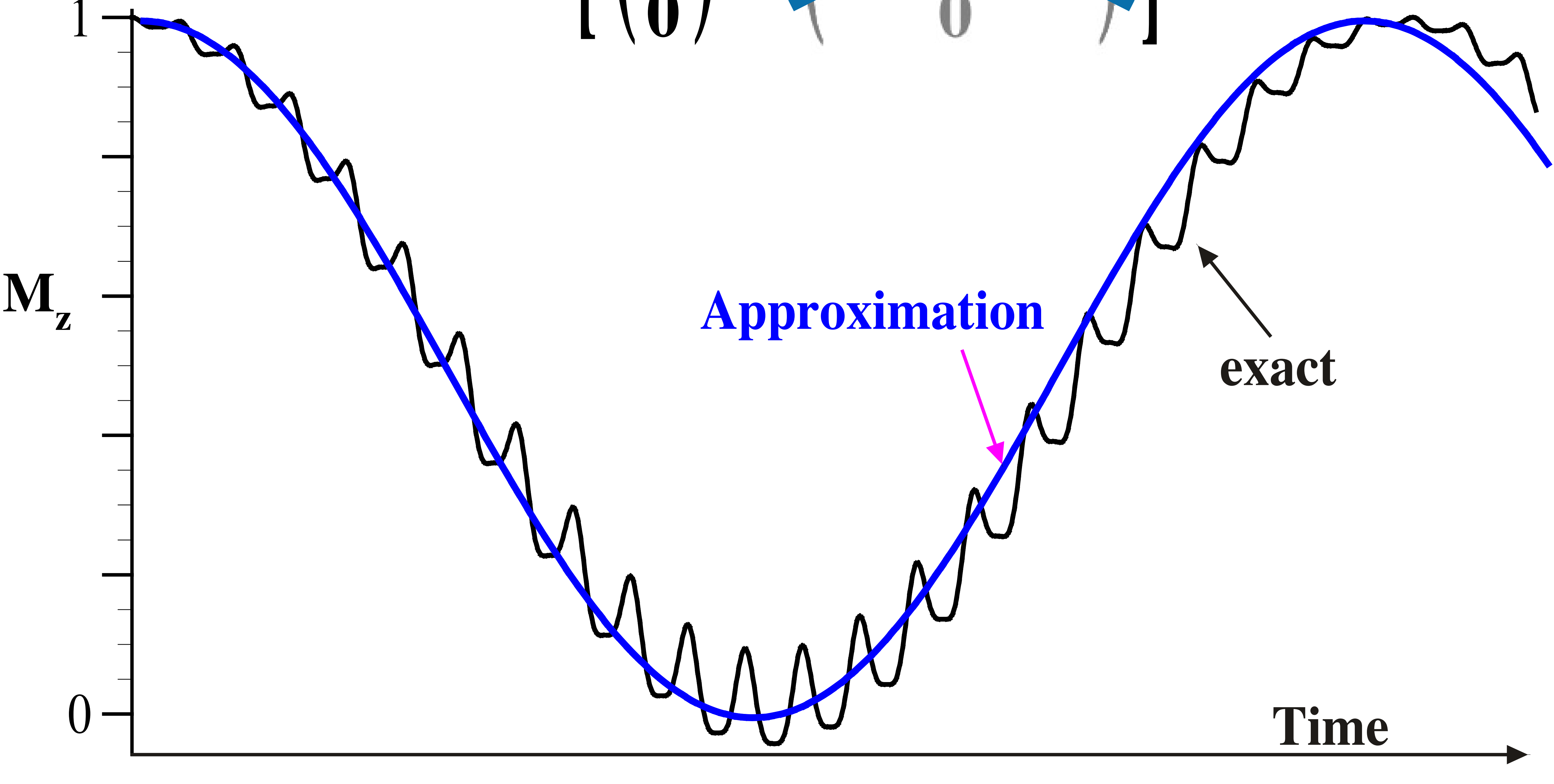
z-component of magnetic field is reduced by ω/γ

x-component given by RF field

Arbitrary directions are possible by adjusting frequency and phase of RF field

Rotating Wave Approximation

$$\vec{B}_1^r = B_1\left[\begin{pmatrix}1\\0\\0\end{pmatrix} + \begin{pmatrix}\cos(2\omega t)\\-\sin(2\omega t)\\0\end{pmatrix}\right]$$

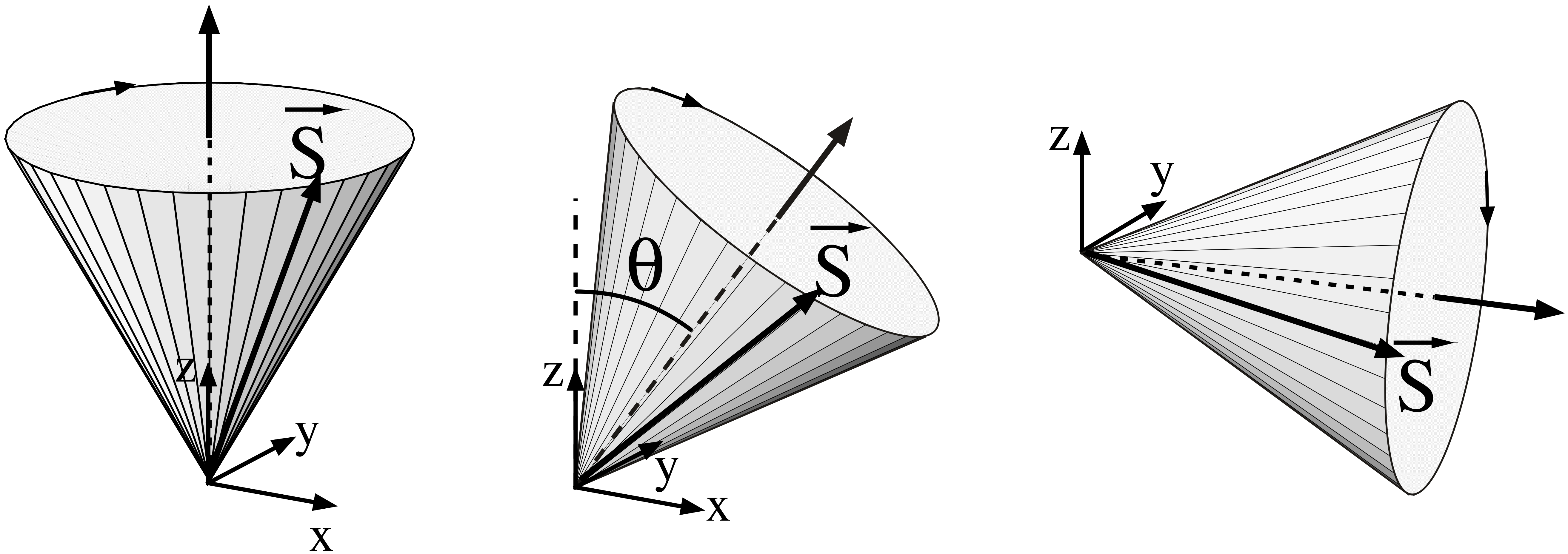


Precession: Special Cases

a) $\Delta\omega_0 \neq 0$, $\omega_1 = 0$

b) $\Delta\omega_0 \neq 0$, $\omega_1 \neq 0$

c) $\Delta\omega_0 = 0$, $\omega_1 \neq 0$

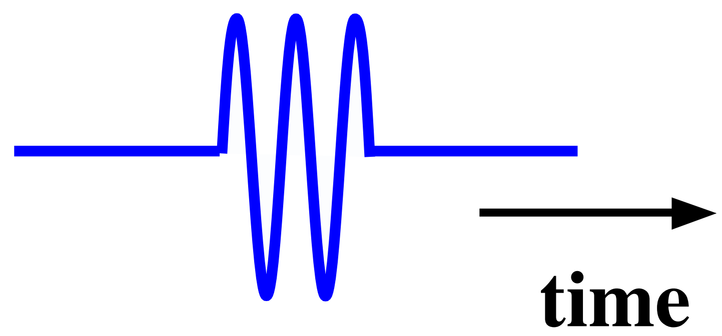


Free Precession

Resonant Excitation

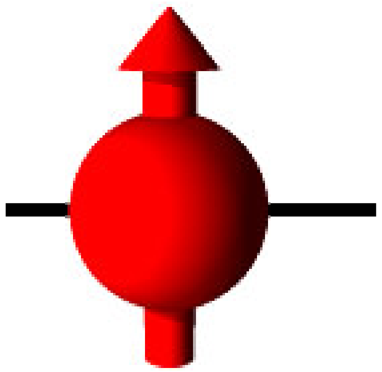
RF Pulses

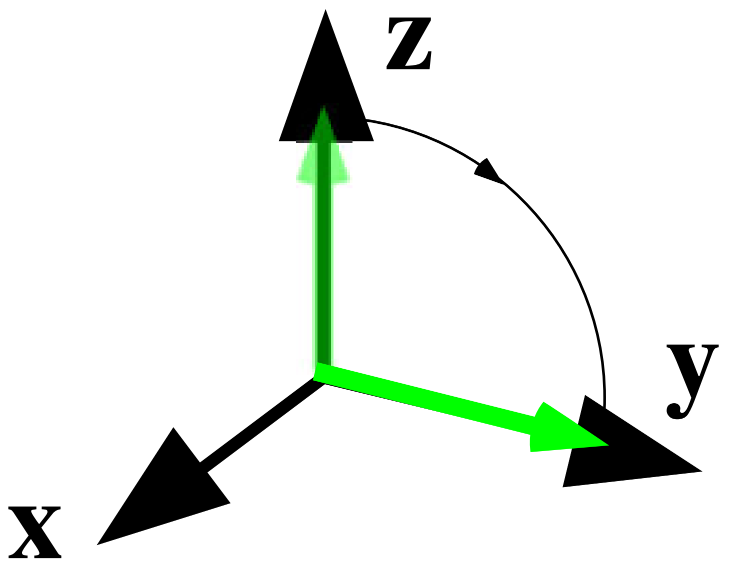
"π/2 pulse"

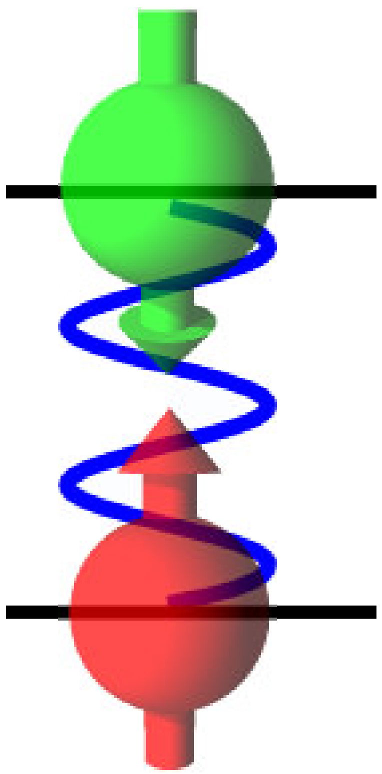


Choose $\omega_{eff}\,\tau = \pi/2$

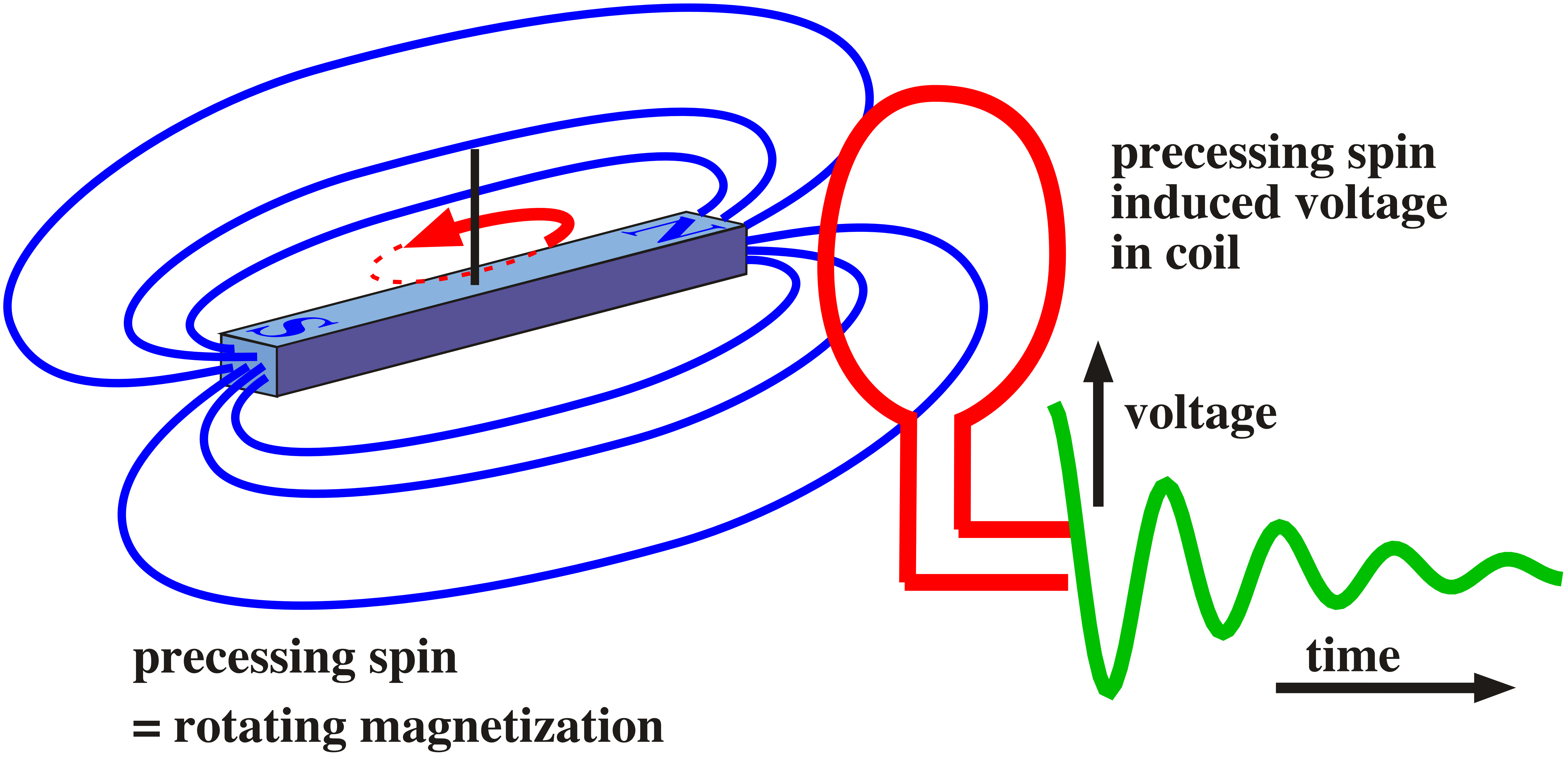
e.g. $(\frac{\pi}{2})_x$-rotation







Detection of precessing Magnetization by Faraday Effect



Signal

$$s(t) = \frac{\hbar\omega_0^2}{2k_BT}\cos(\omega_0 t)e^{-t/T_2}$$

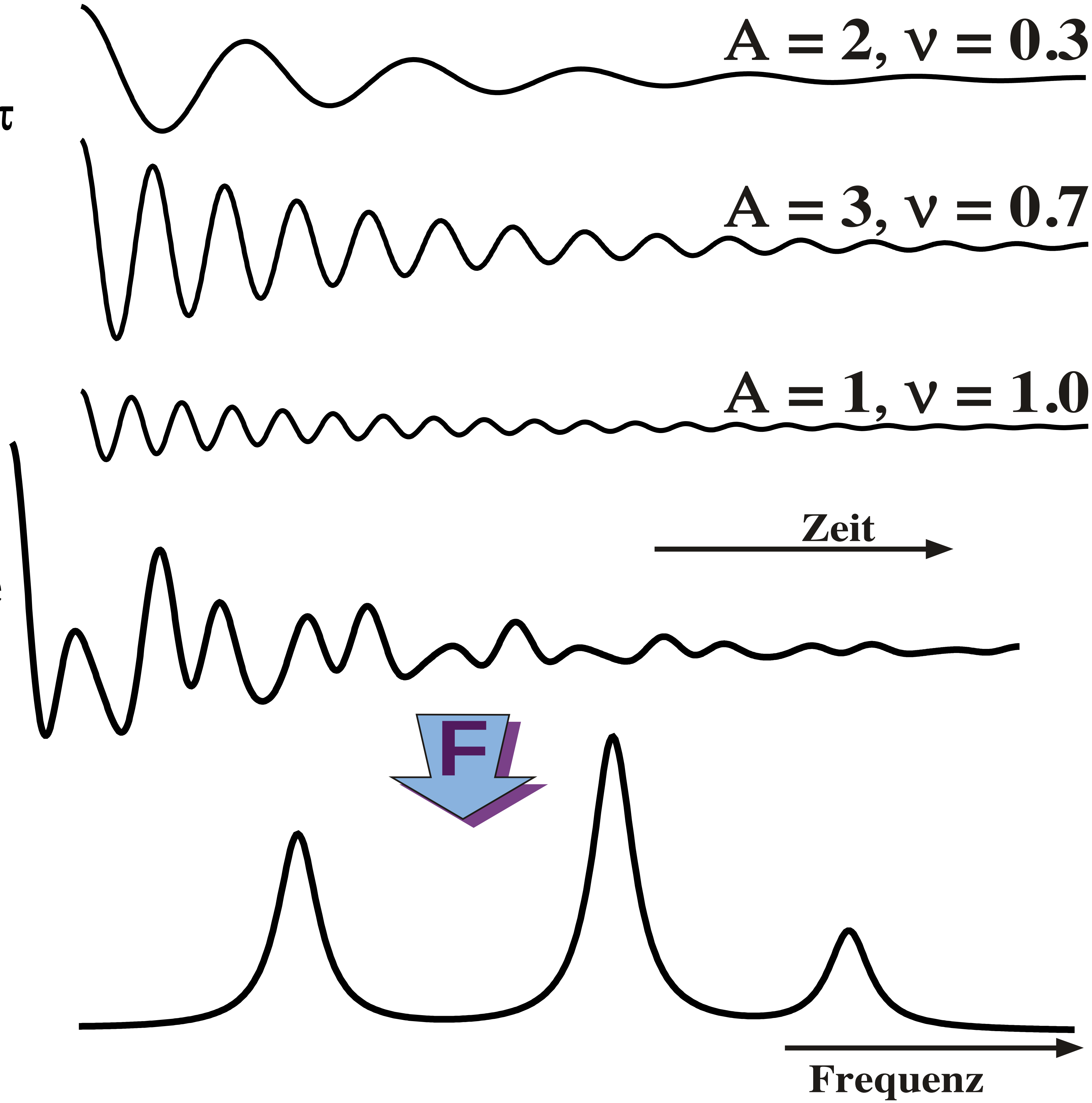
F

$$s(\omega) = \sqrt{\frac{1}{2\pi}}\frac{\hbar\omega_0^2}{4k_BT}\frac{T_2}{1+(\omega-\omega_0)^2T_2^2}$$

$$= \sqrt{\frac{1}{2\pi}}\frac{\hbar\omega_0^2}{4k_BT}\frac{1/T_2}{1/T_2^2+(\omega-\omega_0)^2}$$

Fouriertransformation

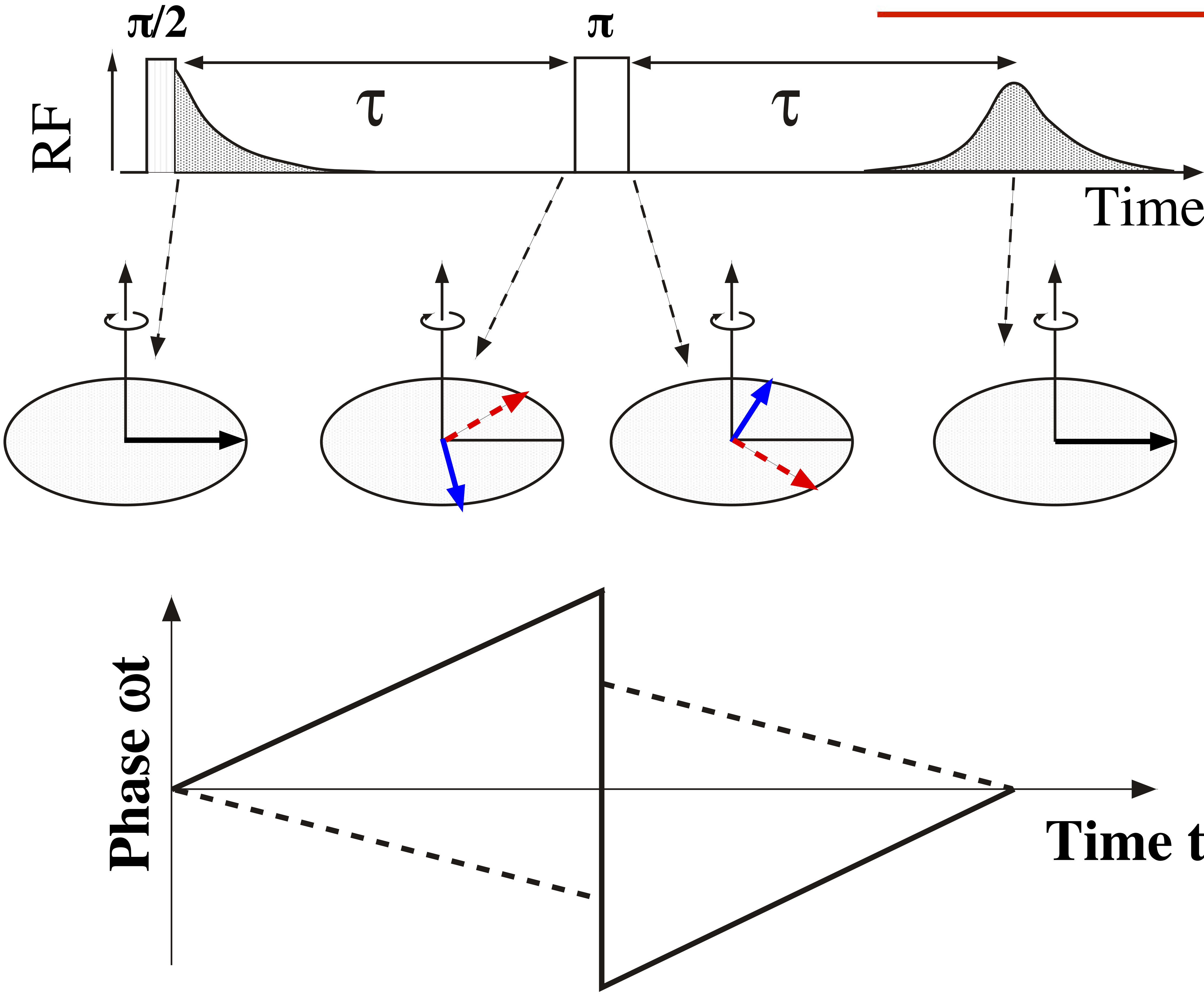
$$s_{ij}(t) = A_{ij}\, e^{i\omega_{ij}\tau}$$



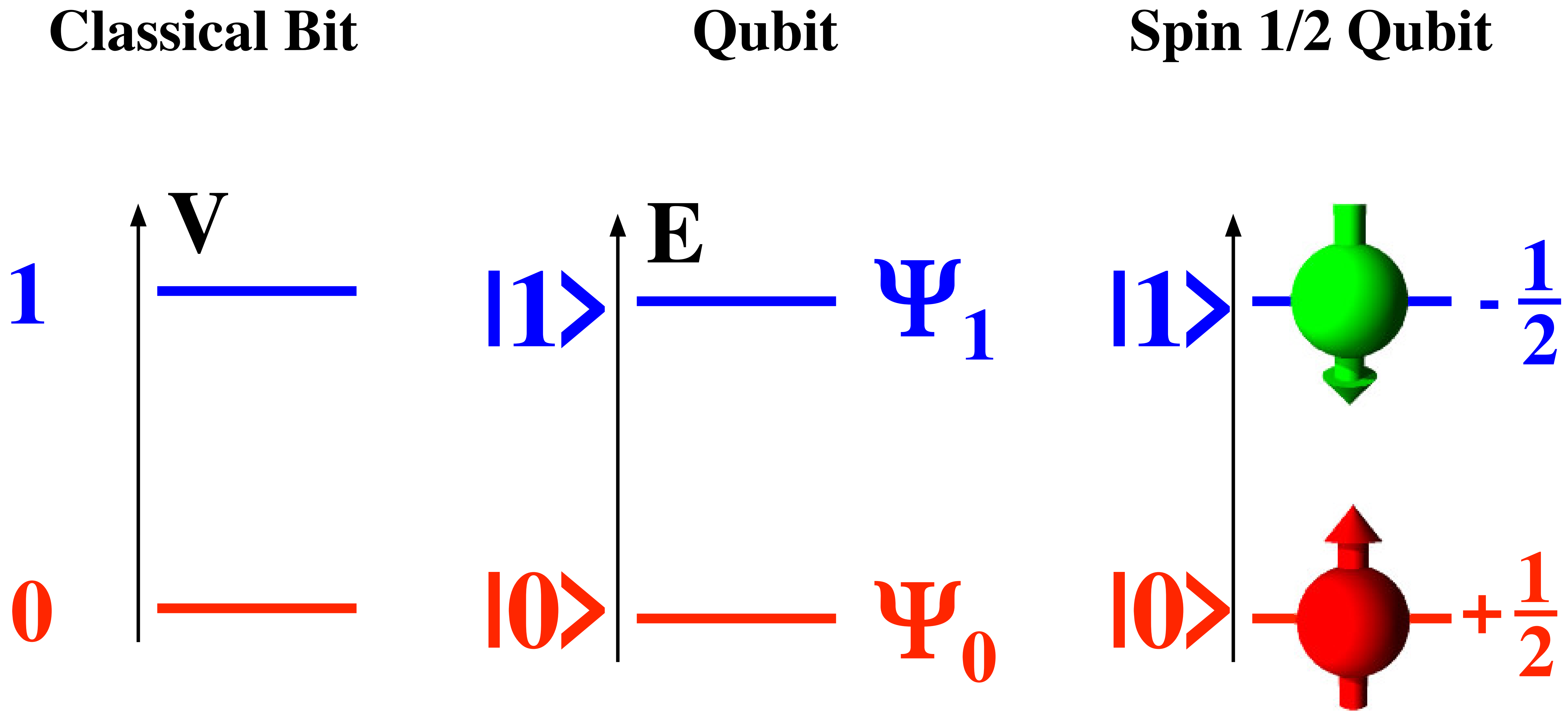
$$\omega_{ij} = (E_i - E_j)/\hbar$$

$$A_{ij} \sim |(I_x)_{ij}|^2$$

Refocusing



Spin 1/2 as Qubit



Qubit as Spin 1/2

JOURNAL OF APPLIED PHYSICS VOLUME 28, NUMBER 1 JANUARY, 1957

Geometrical Representation of the Schrödinger Equation for Solving Maser Problems

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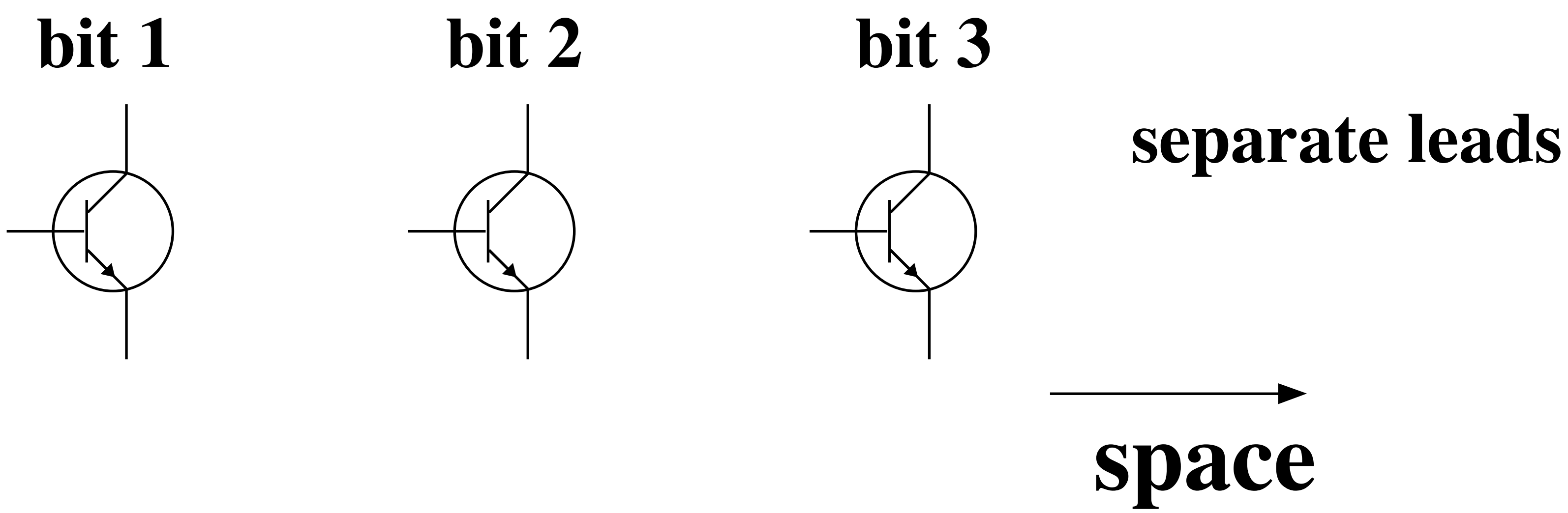
(Received September 18, 1956)

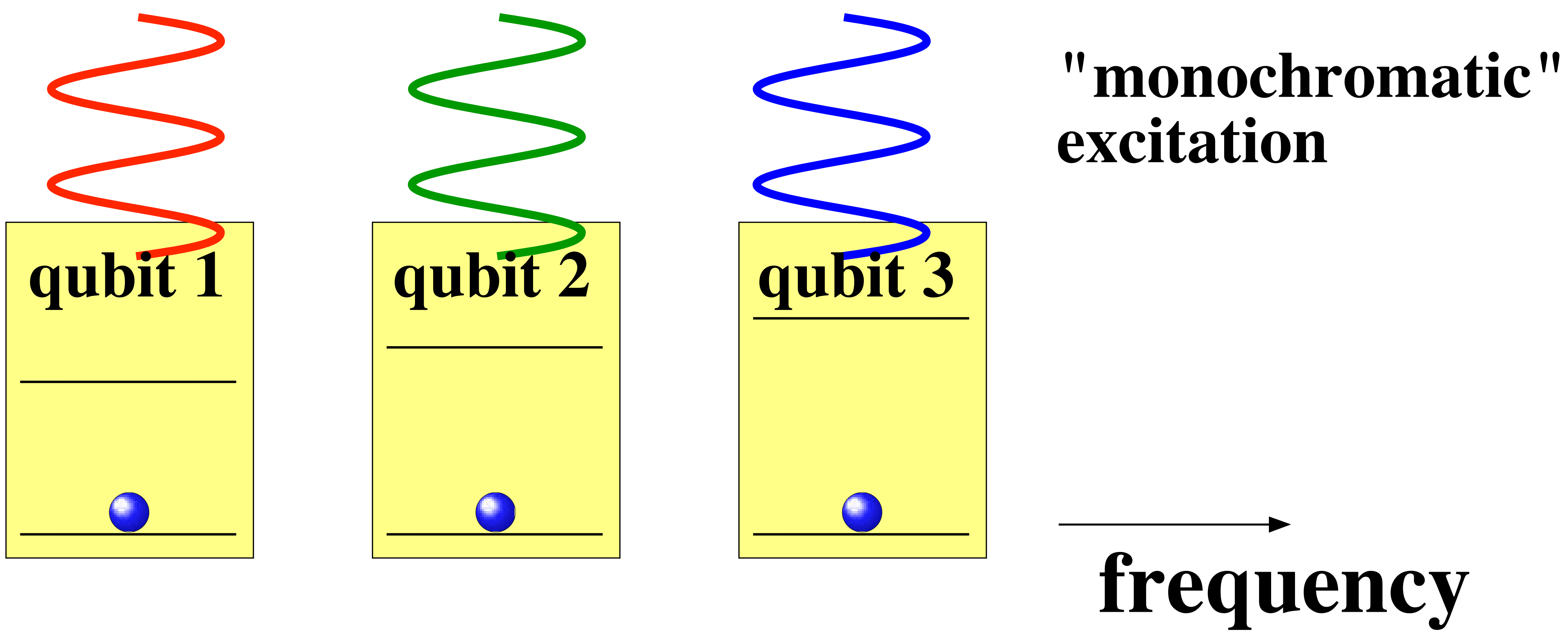
A simple, rigorous geometrical representation for the Schrödinger equation is developed to describe the behavior of an ensemble of two quantum-level, noninteracting systems which are under the influence of a perturbation. In this case the Schrödinger equation may be written, after a suitable transformation, in the form of the real three-dimensional vector equation $d\mathbf{r}/dt=\boldsymbol{\omega}\times\mathbf{r}$, where the components of the vector $\mathbf{r}$ uniquely determine ψ of a given system and the components of $\boldsymbol{\omega}$ represent the perturbation. When magnetic interaction with a spin $\frac{1}{2}$ system is under consideration, "r" space reduces to physical space. By analogy the techniques developed for analyzing the magnetic resonance precession model can be adapted for use in any two-level problems. The quantum-mechanical behavior of the state of a system under various different conditions is easily visualized by simply observing how $\mathbf{r}$ varies under the action of different types of $\boldsymbol{\omega}$. Such a picture can be used to advantage in analyzing various MASER-type devices such as amplifiers and oscillators. In the two illustrative examples given (the beam-type MASER and radiation damping) the application of the picture in determining the effect of the perturbing field on the molecules is shown and its interpretation for use in the complex Maxwell's equations to determine the reaction of the molecules back on the field is given.

Addressing Qubits

Solid-State Computer

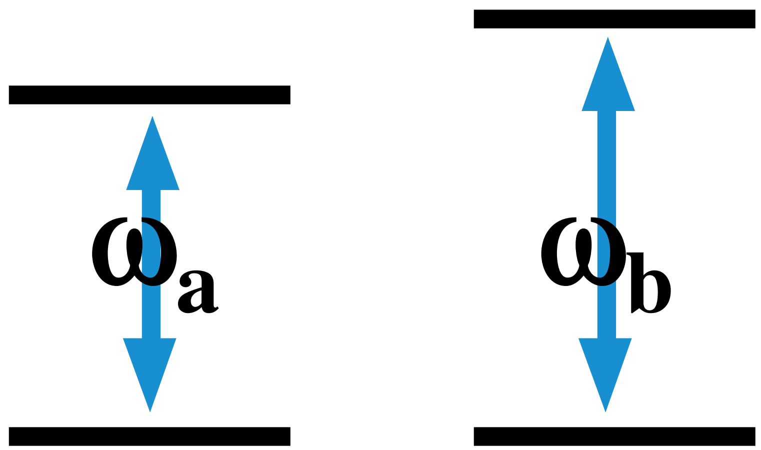


Liquid-State NMR Quantum Computer



Selective Excitation

Qubit a **Qubit b**



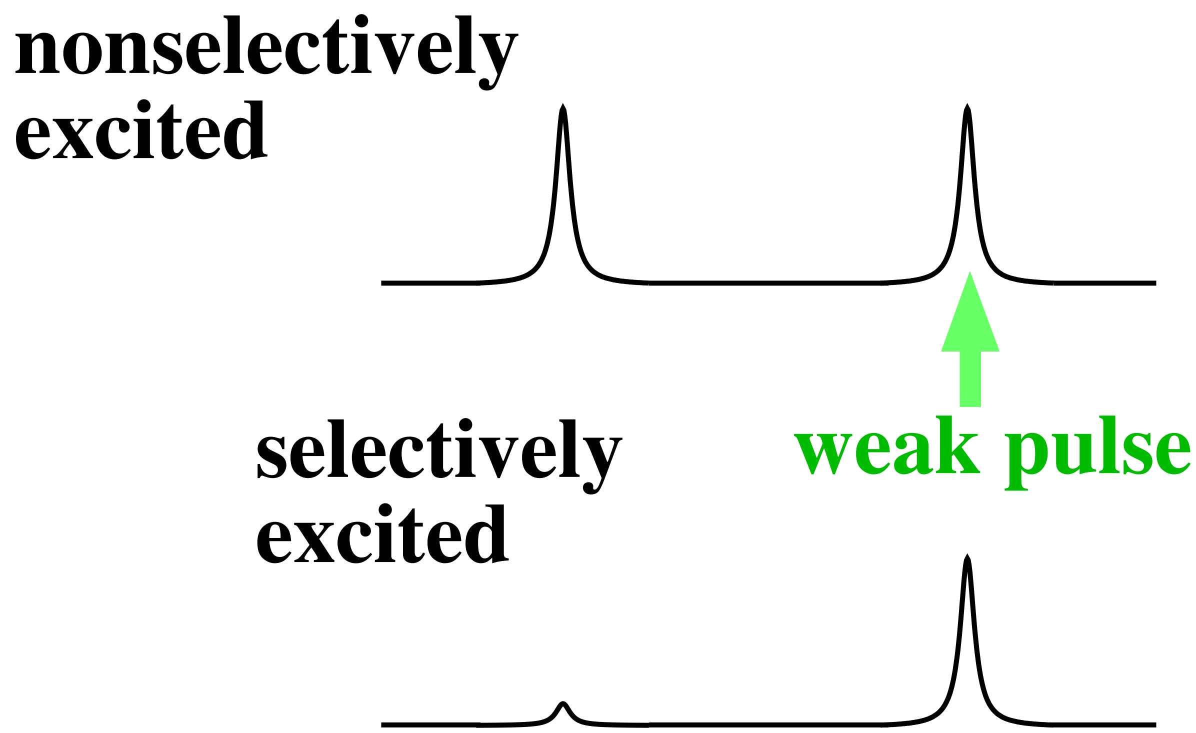
Different qubits = different nuclear isotopes

e.g. ^{1}H, ^{13}C, ^{19}F

Resonance frequencies @ 14 T: 600 MHz, 151 MHz, 565 MHz

Condition for selective excitation:

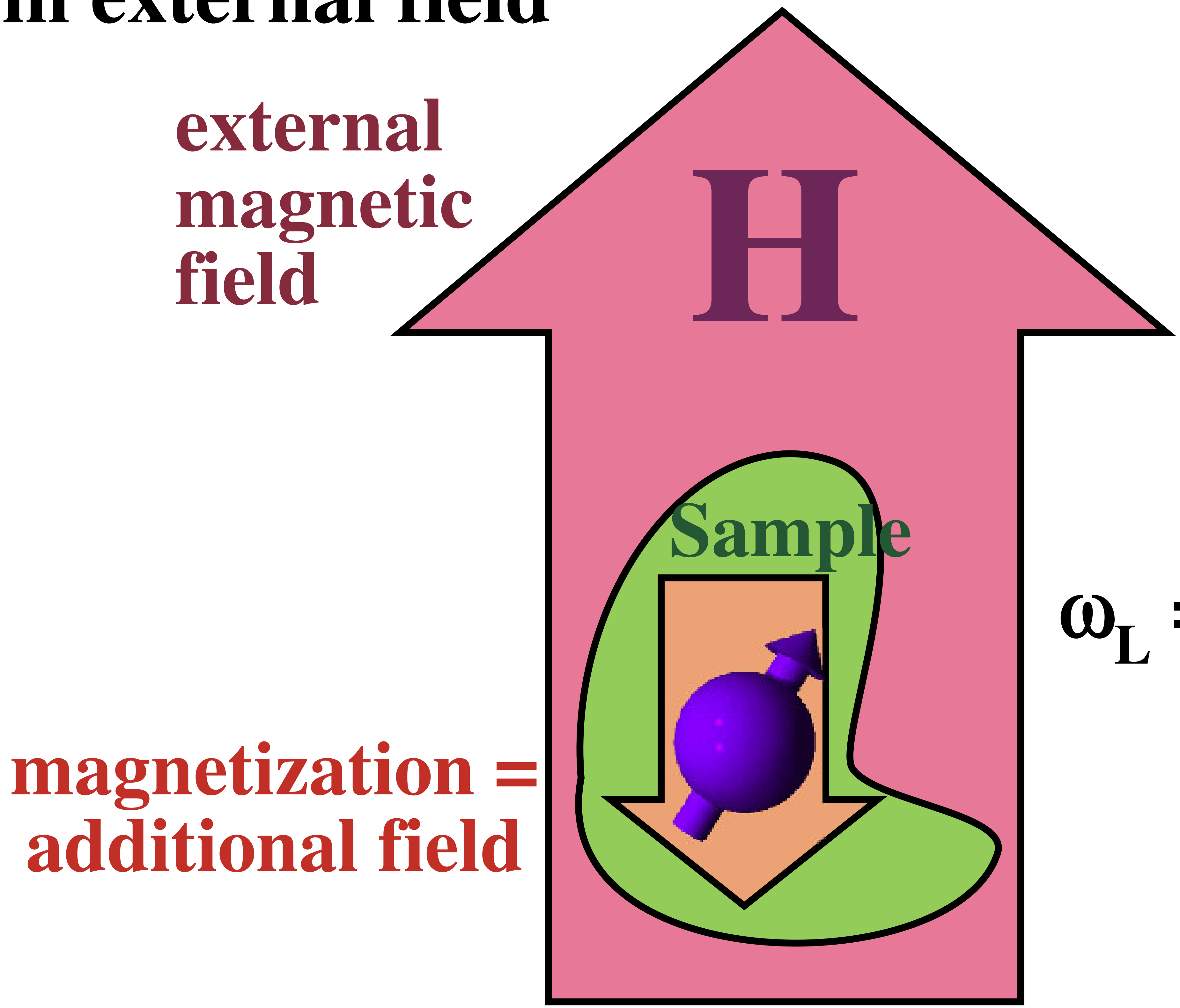
$$|\omega_a - \omega_b|\ \tau \gg 1$$



RF pulses excite only one isotope

Chemical Shift

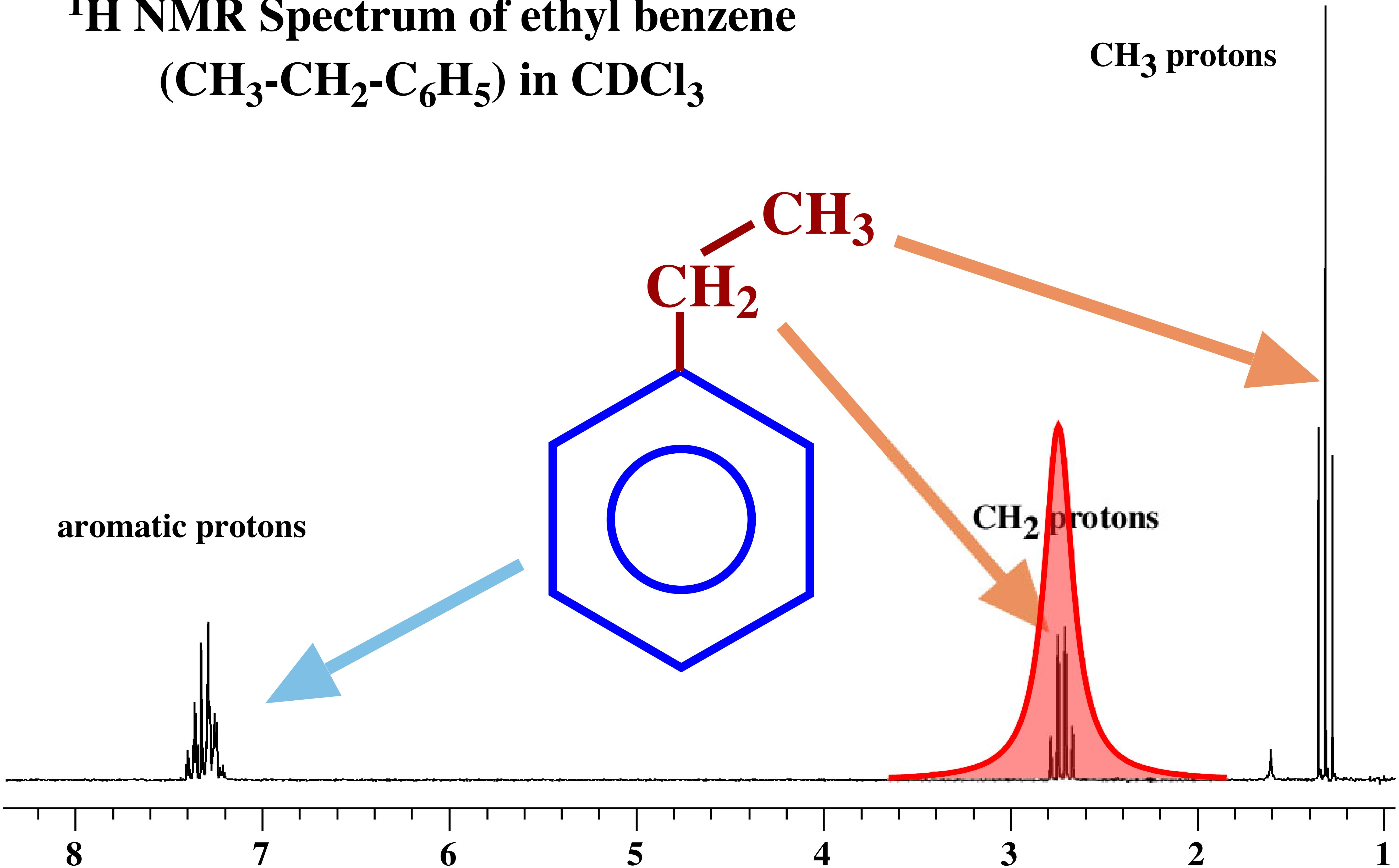
Local fields differ from external field



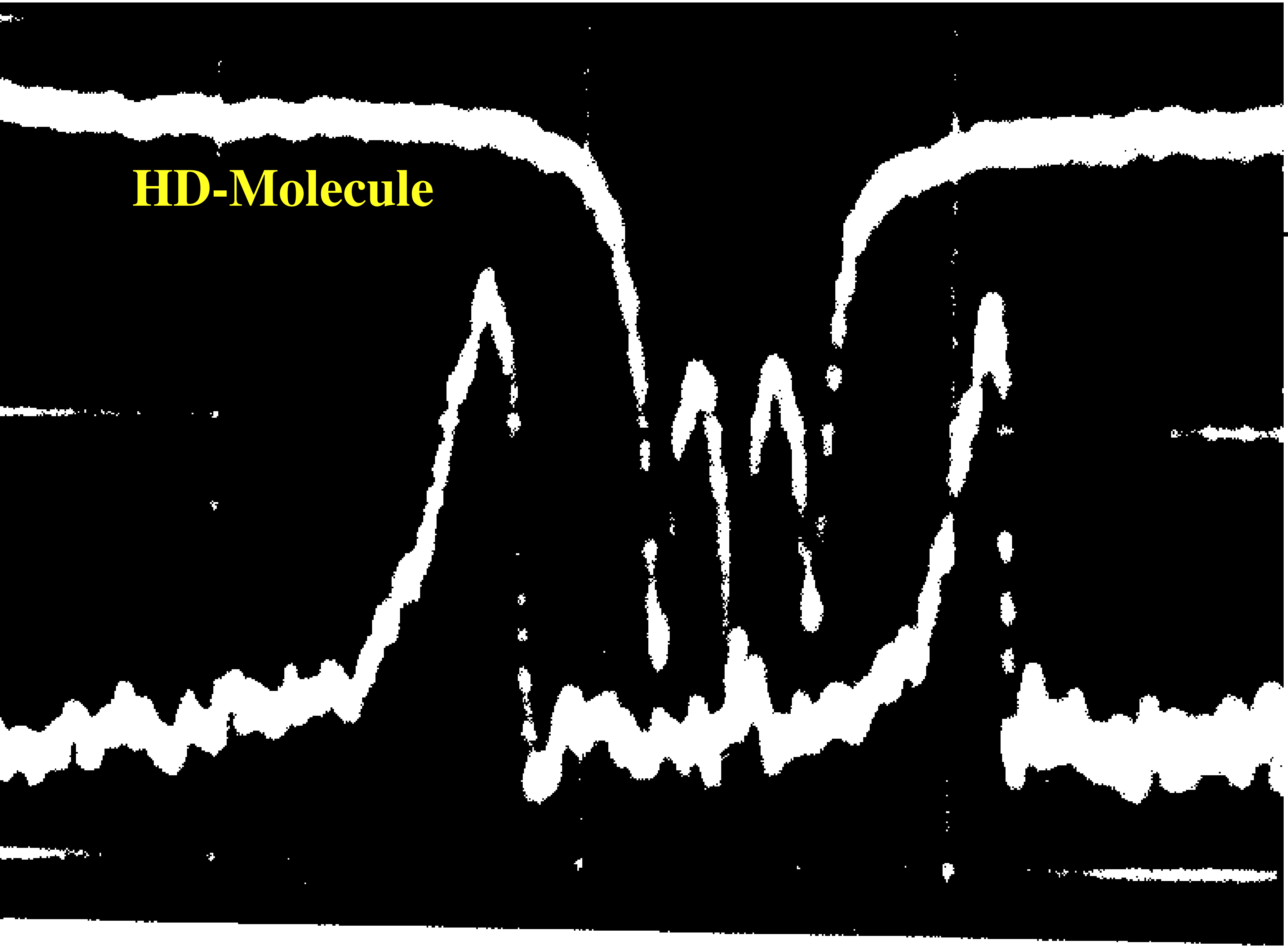
$$\omega_L = \gamma B_{loc}$$

Example

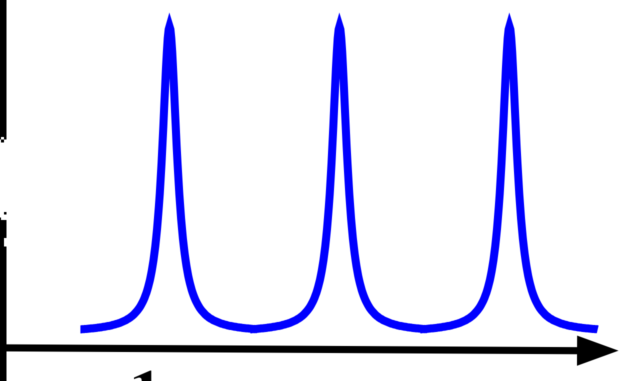
^{1}H NMR Spectrum of ethyl benzene (CH_3-CH_2-C_6H_5) in $CDCl_3$

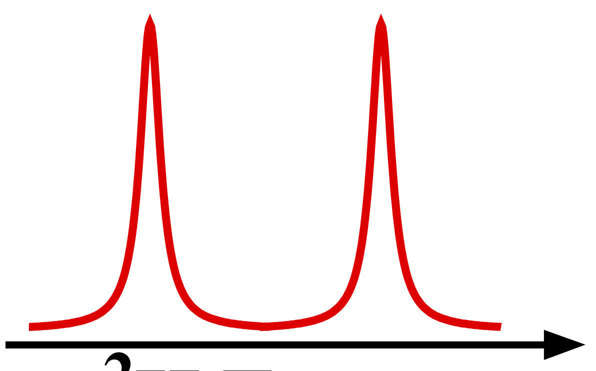


Spin-Spin Couplings

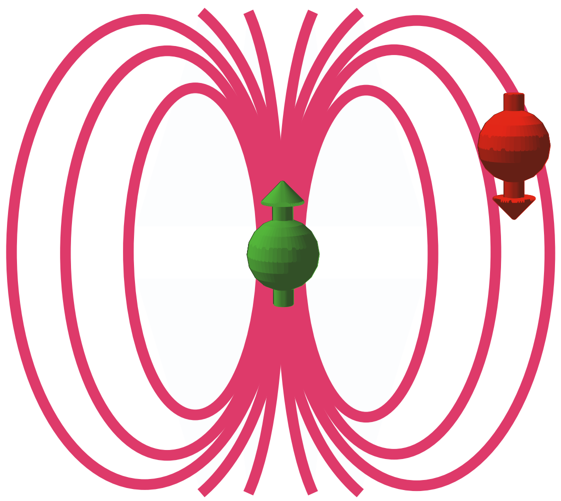


. XI, 2. Simultaneous display of deuteron and proton resonances in HD. The proton trace is inverted.

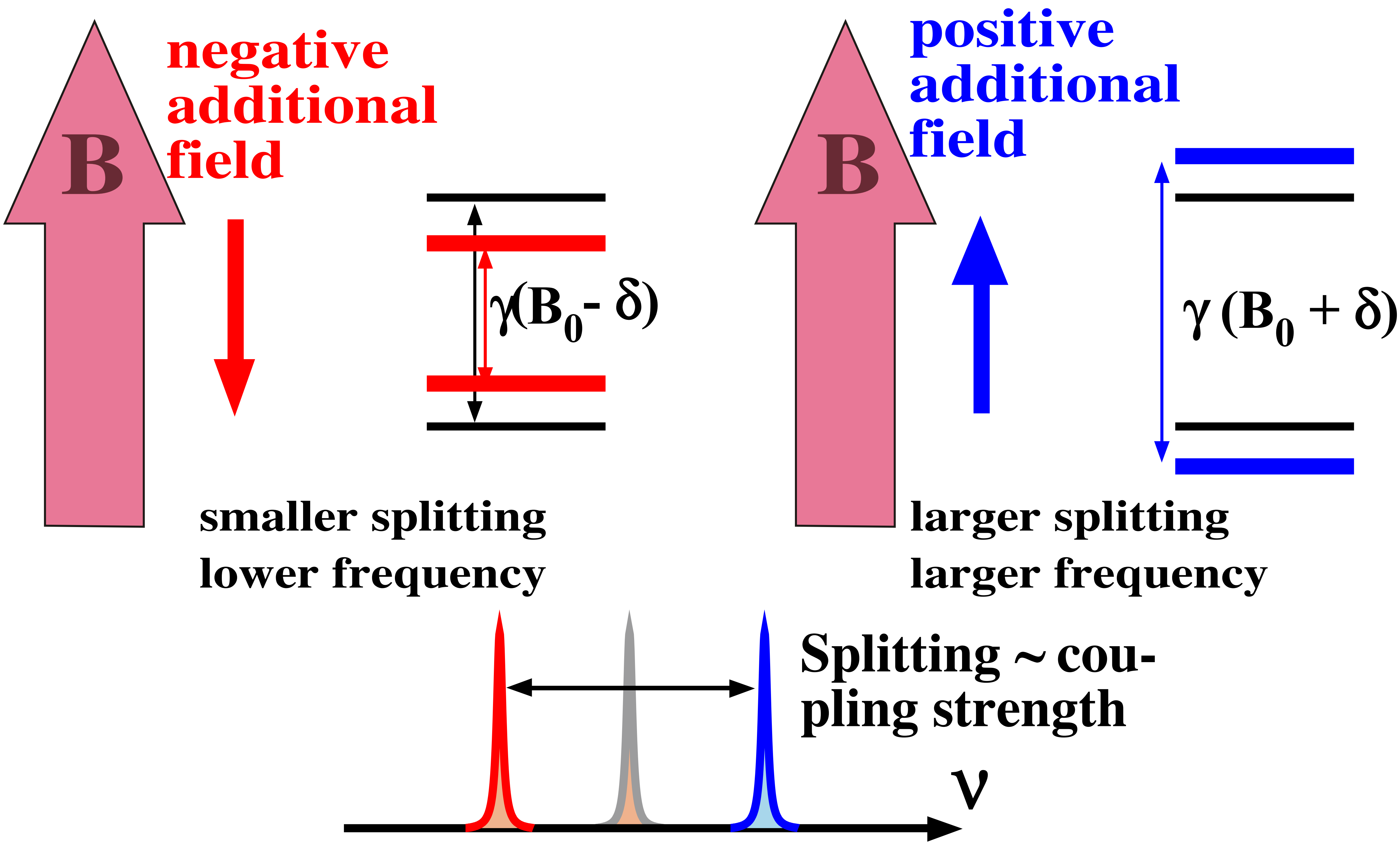




Couplings as Effective Fields



Coupling partner : Spin 1/2



Dipole - Dipole Coupling

in a strong magnetic field

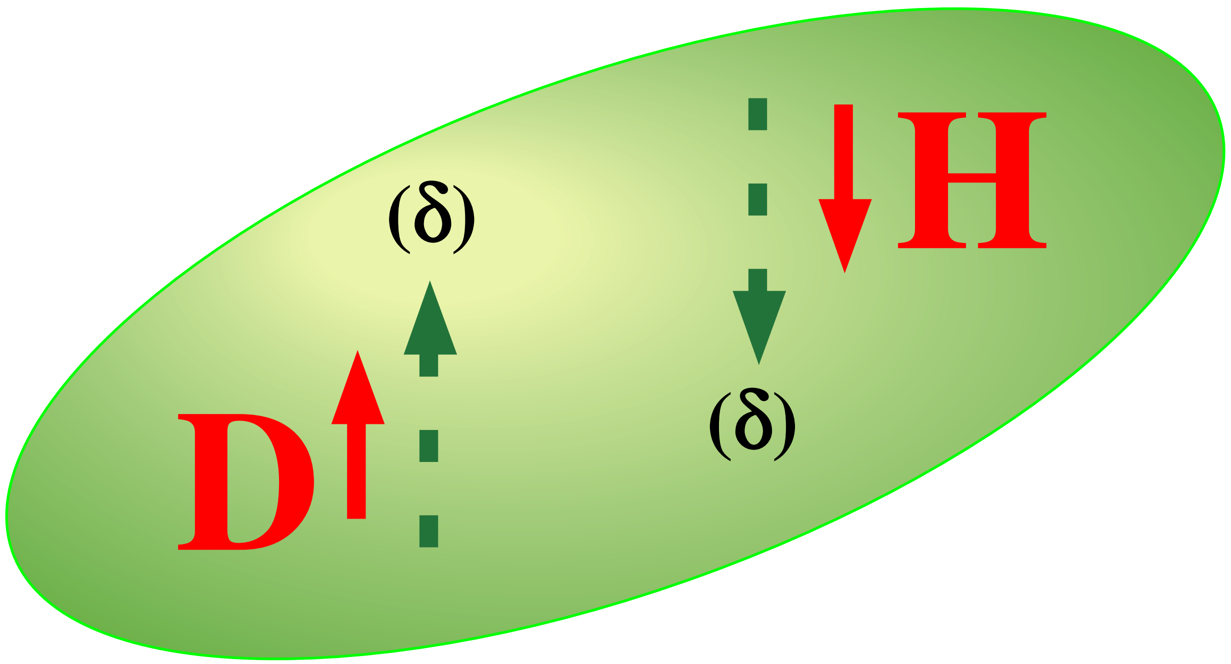
$$E_{dd} = \frac{\mu_0}{4\pi r_{12}^3}\,\mu_1\mu_2(1\text{-}3\cos^2\theta)$$

averaged to 0 in isotropic liquids

Indirect Coupling

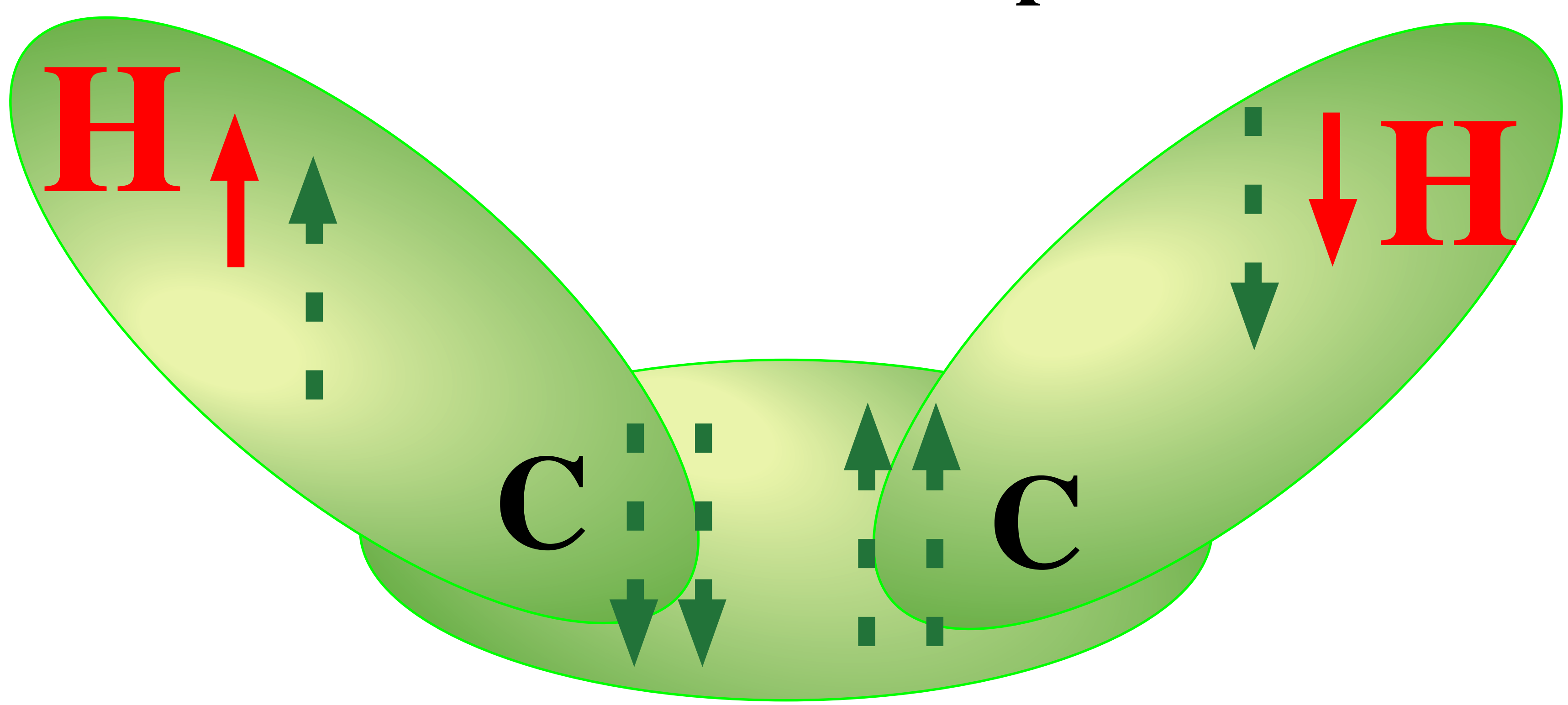
Partial polarisation of electrons in chemical bonds by hyperfine coupling

$$E = -J\,\vec{\mu}_1 \cdot \vec{\mu}_2$$



Multiple bonds

The Pauli - principle causes antiparallel orientation of electrons



Coupling Hamiltonian

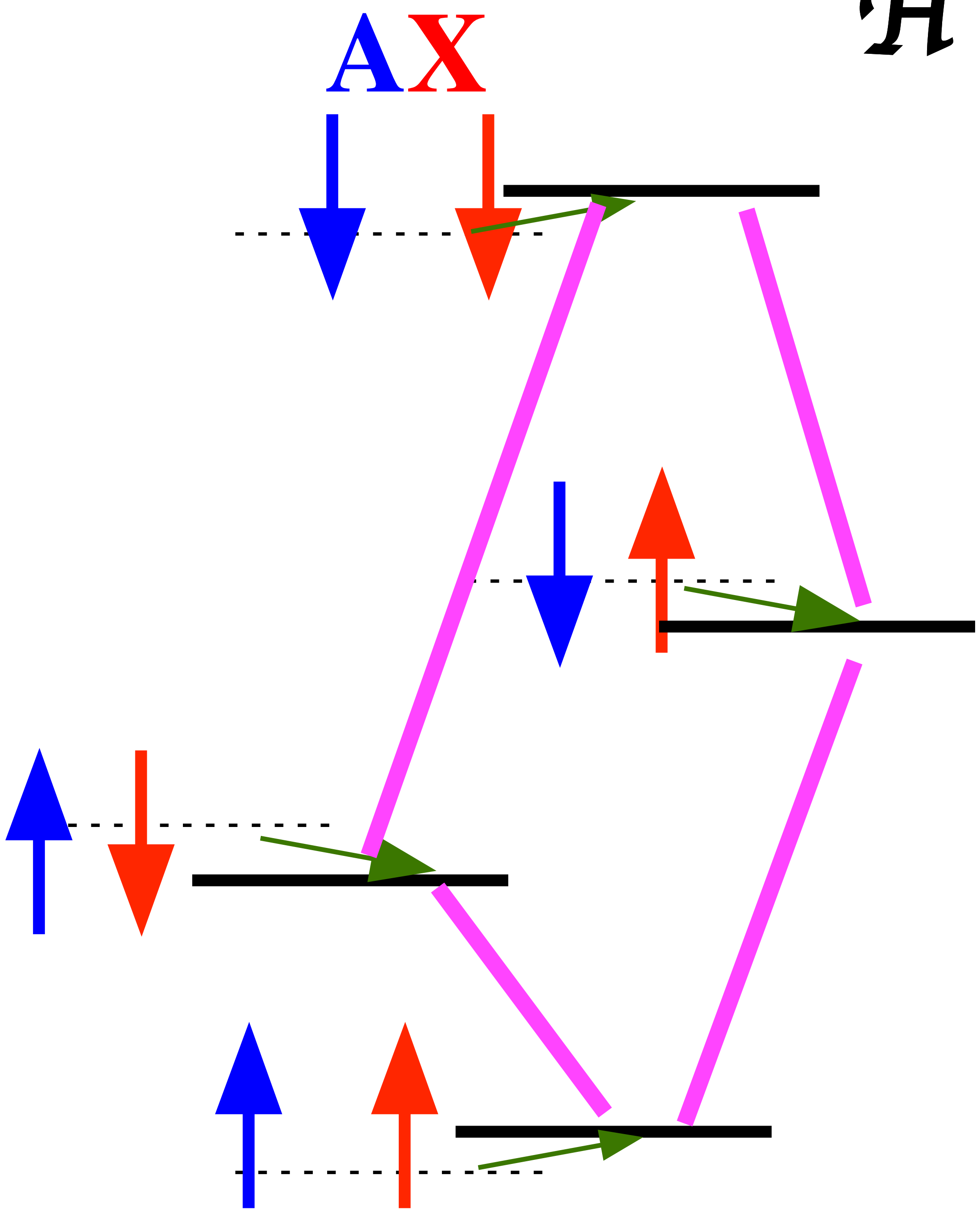
$$\mathcal{H} = \mathcal{H}_z + \mathcal{H}_{AX} = -\omega_A \mathbf{A}_z - \omega_X \mathbf{X}_z + d\mathbf{A}_z \mathbf{X}_z =$$

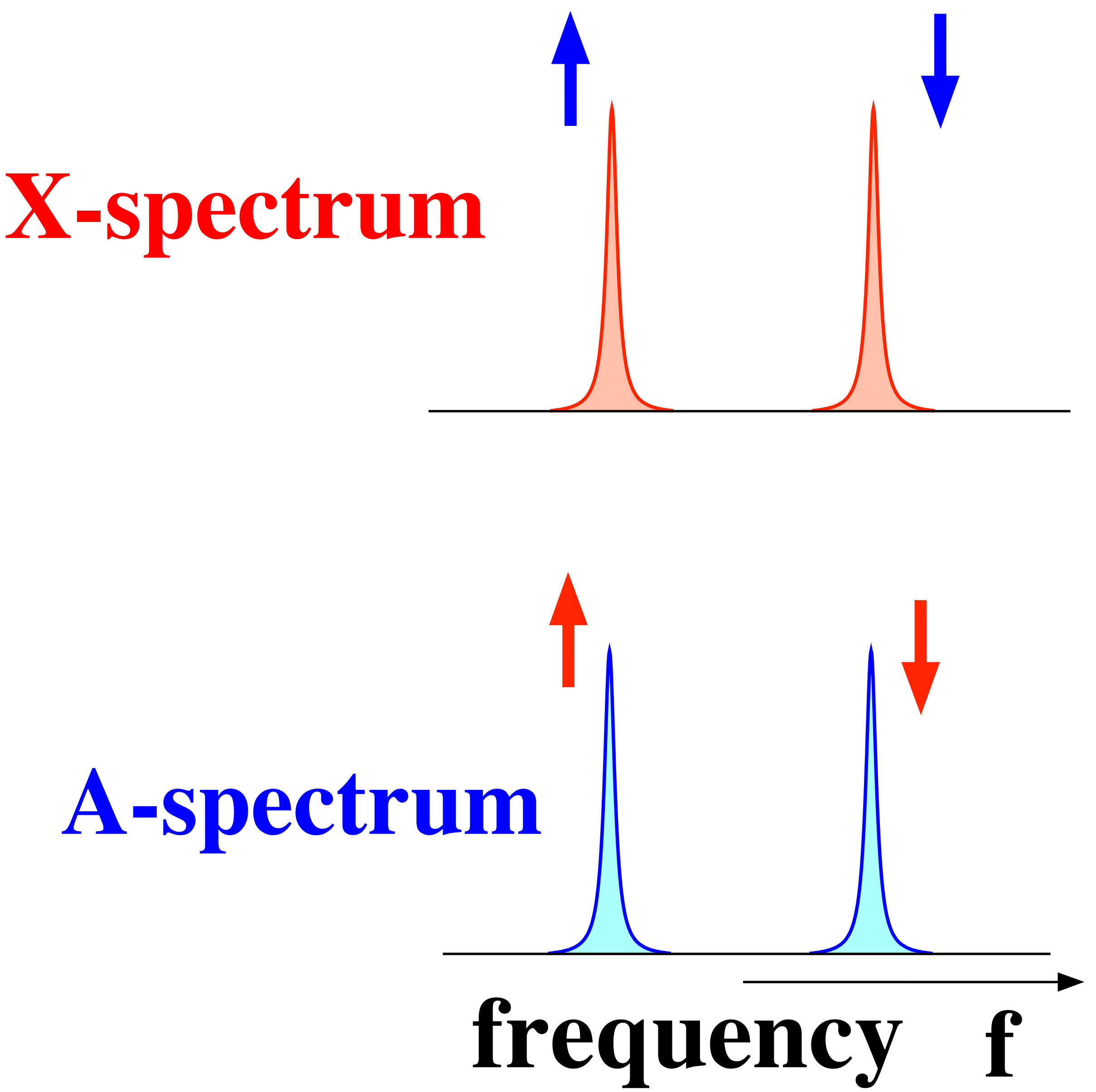
$$= \frac{1}{2}\begin{pmatrix} -\omega_A - \omega_X + \frac{d}{2} & & & \\ & -\omega_A + \omega_X - \frac{d}{2} & & \\ & & \omega_A - \omega_X - \frac{d}{2} & \\ & & & \omega_A + \omega_X + \frac{d}{2} \end{pmatrix}$$

Coupled Spin Systems

Coupled 2-spin system

$$\mathcal{H} = -\omega_A A_z - \omega_X X_z + d\, A_z X_z$$

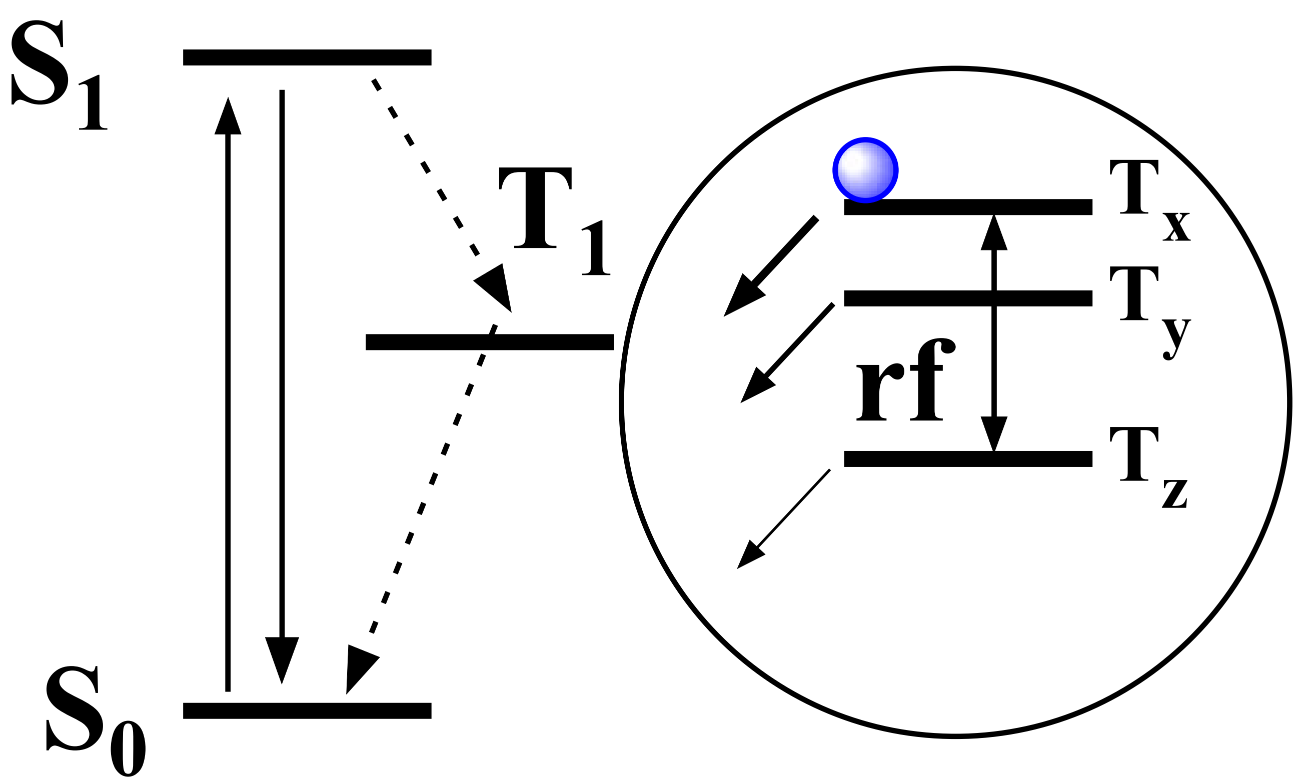




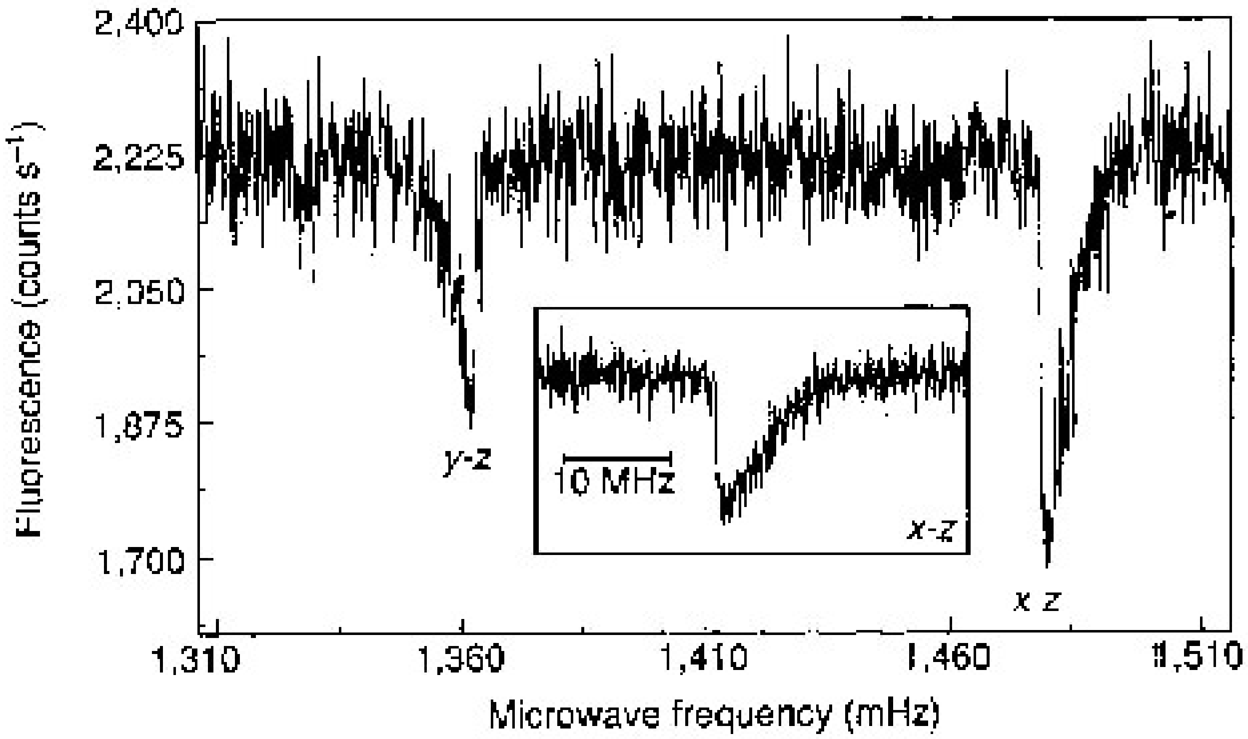
Single Spin Detection

Not possible by conventional MR, but:

ODMR: Principle



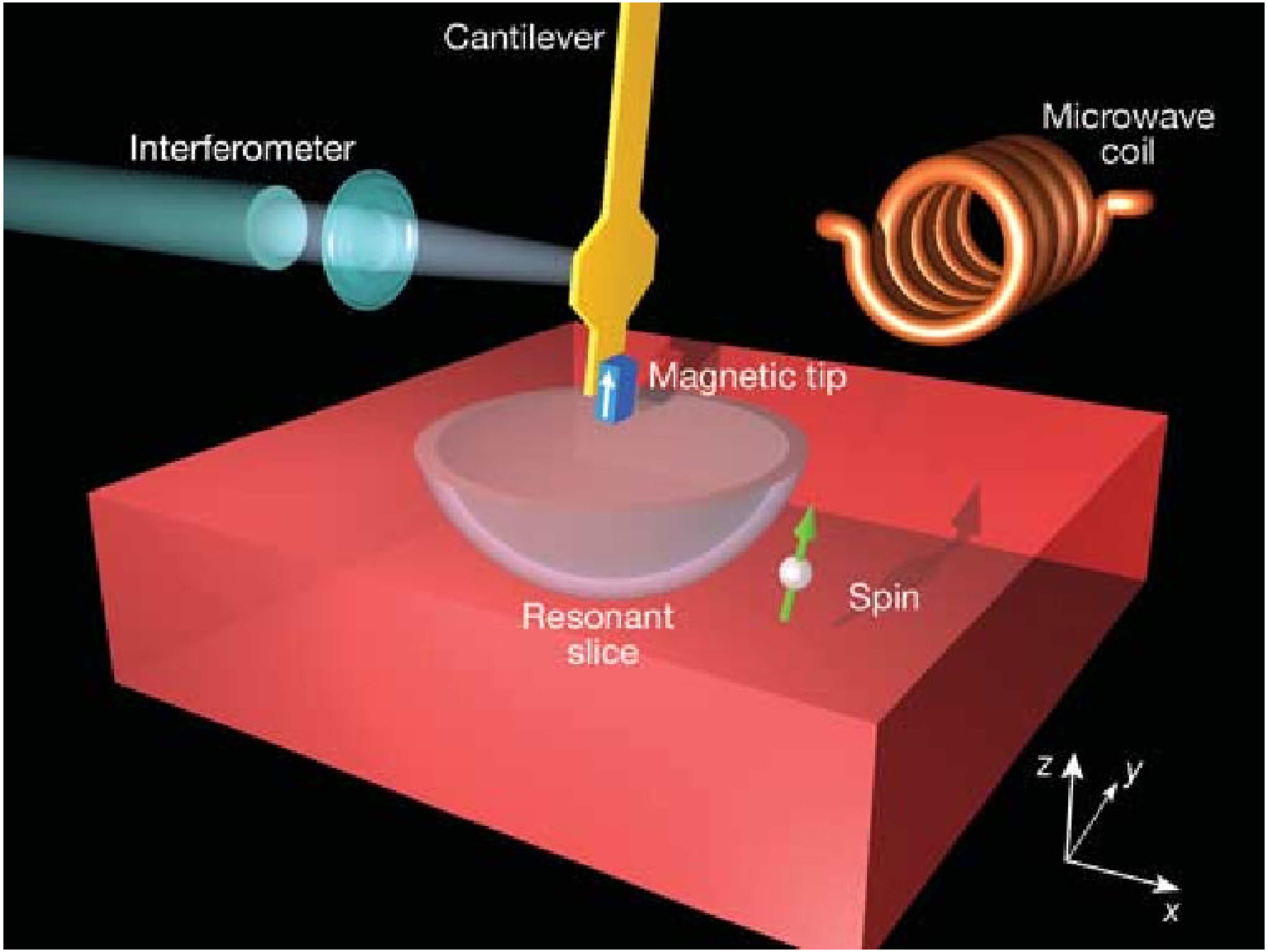
Result from pentacene



J. Köhler, J.A.J.M. Disselhorst, M.C.J.M. Donckers, E.J.J. Groenen, J. Schmidt, and W.E. Moerner, 'Magnetic resonance detection of a single molecular spin', Nature 363, 242 (1993).

J. Wrachtrup, C.v. Borczyskowski, J. Bernard, M. Orrit, and R. Brown, 'Optical detection of magnetic resonance in a single molecule', Nature 363, 244 (1993).

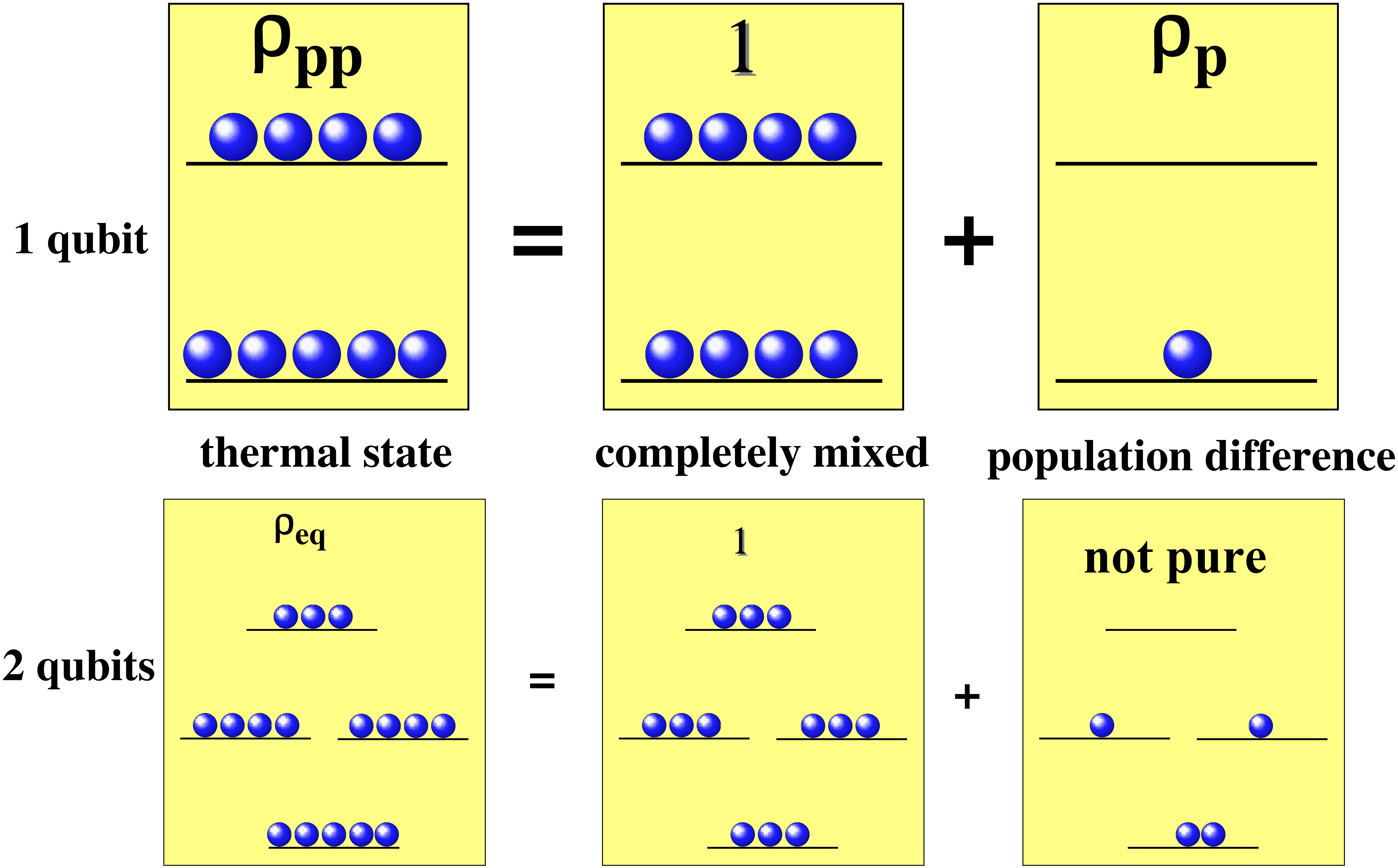
Force Detection



D. Rugar, R. Budakian, H.J. Mamin, and B.W. Chui, 'Single spin detection by magnetic resonance force microscopy', Nature 430, 329 (2004).

Room temperature liquids

Mixed States



Pseudopure States

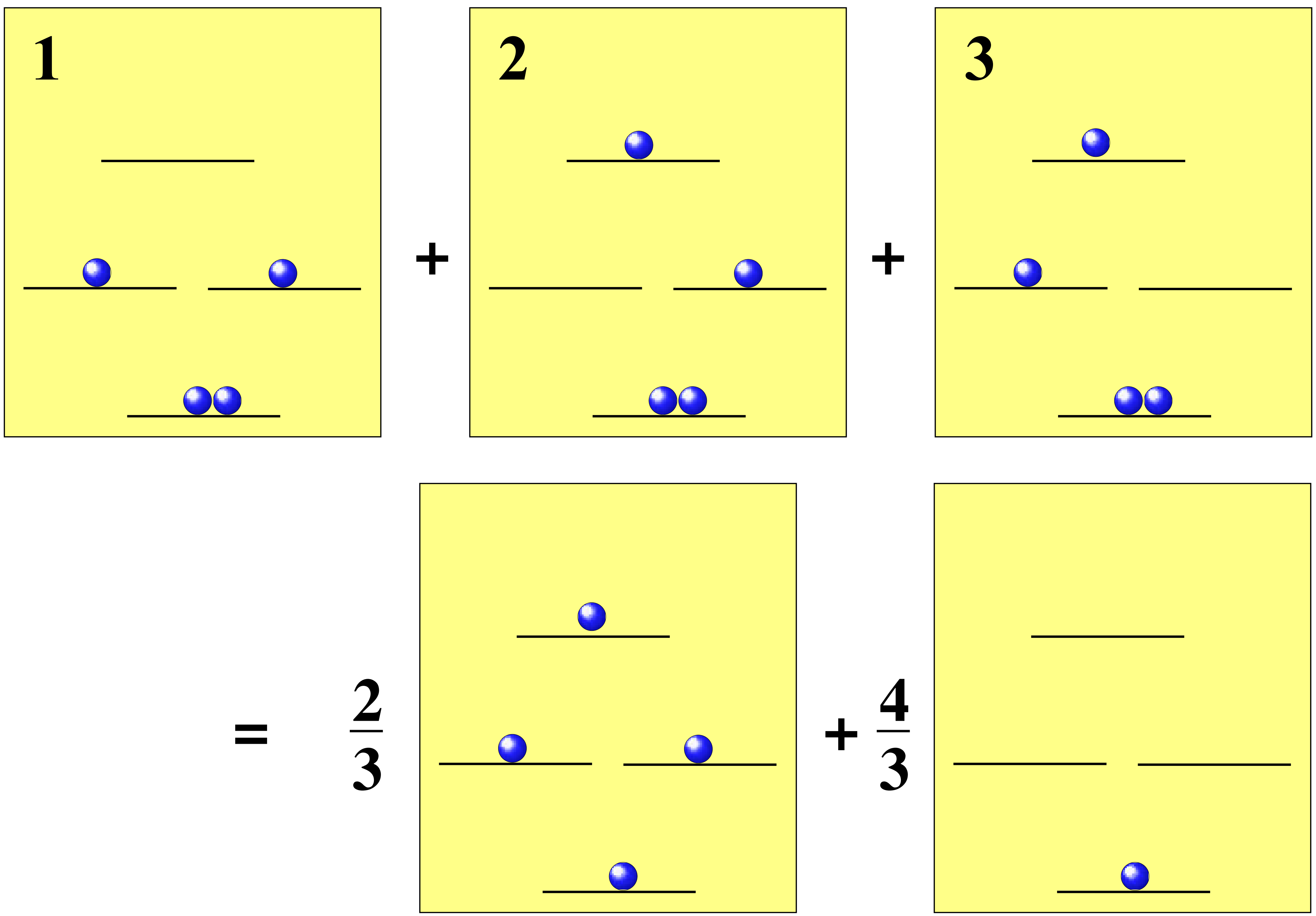
$$\rho_{pp} = \mathbb{1} + \varepsilon\, \rho_p$$

pure state

- **Pseudopure states are** (for all practical purposes) **equivalent to pure states**
- **pp state preparation associated with exponential signal loss**
- **Some algorithms can be applied directly to mixed states**

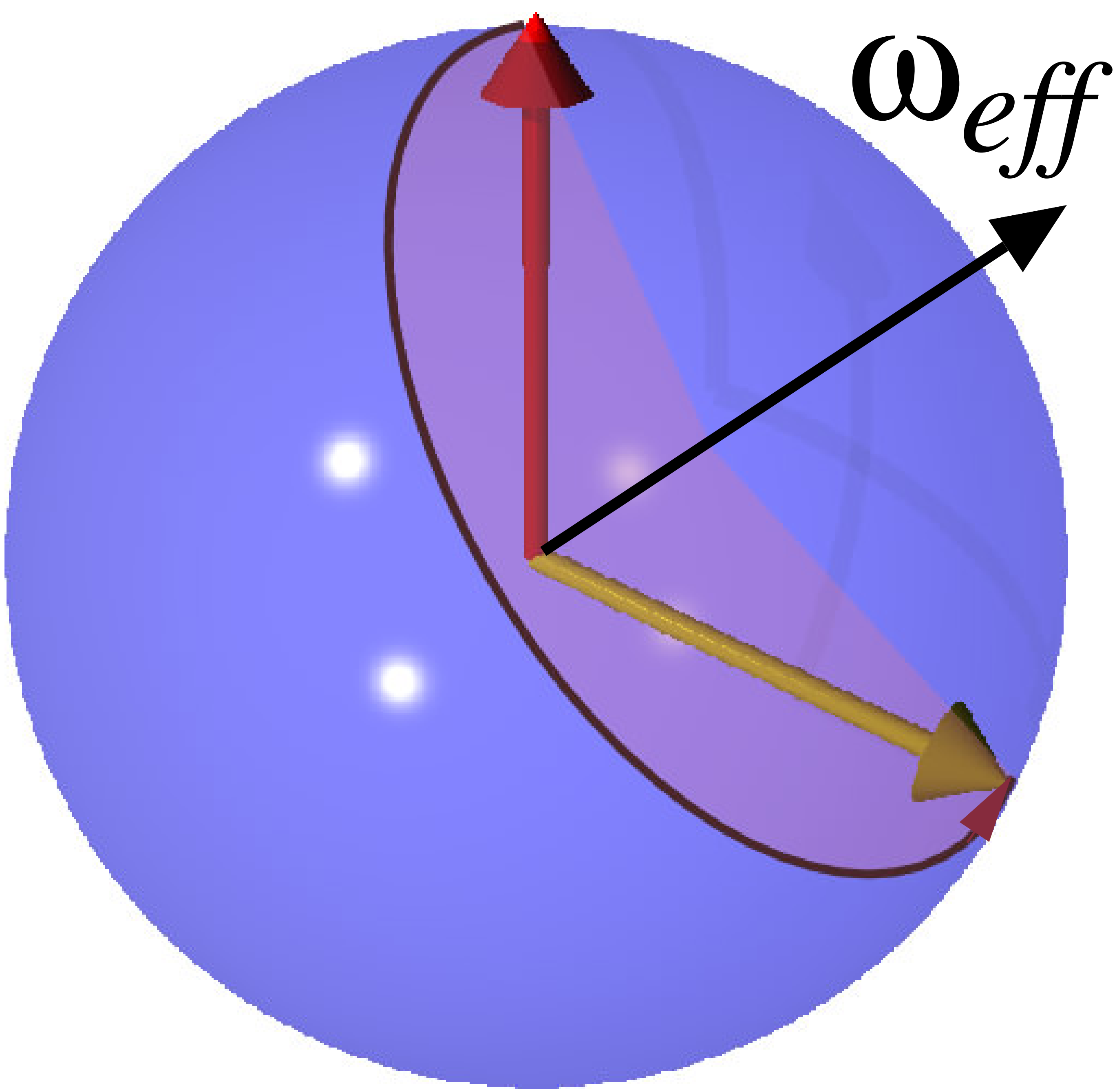
Temporal Labeling

Sum of 3 experiments



Single Qubit Gates

Time evolution of spins =
Larmor precession around effective field



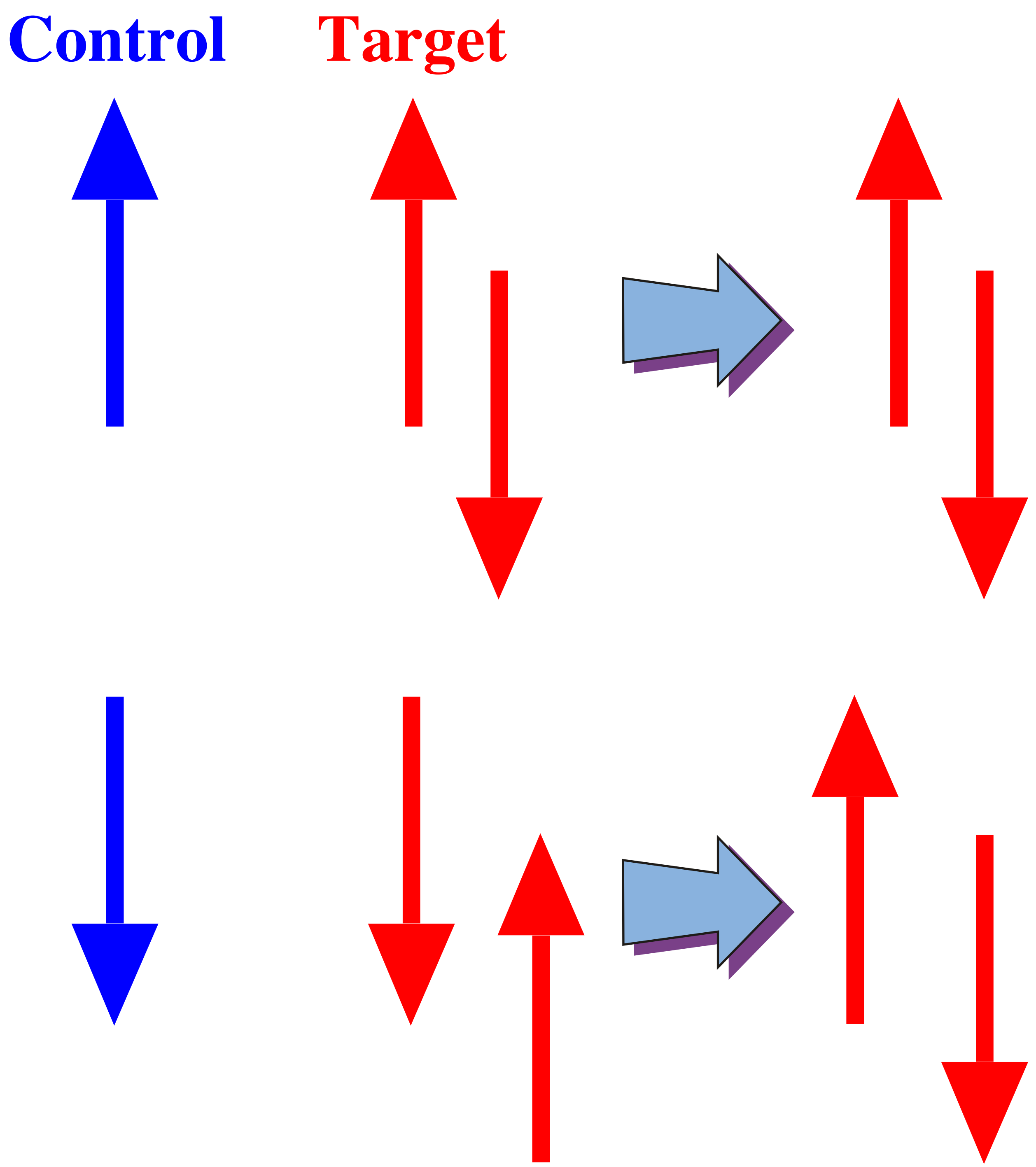
$$U = e^{i\vec{\omega}_{eff}\cdot\vec{I}\tau}$$

arbitrary rotations are possible by appropriate choice of ω_{eff}, τ

Two Qubit Gates

Required for universal quantum computer: 2-qubit gate, e.g. CNOT

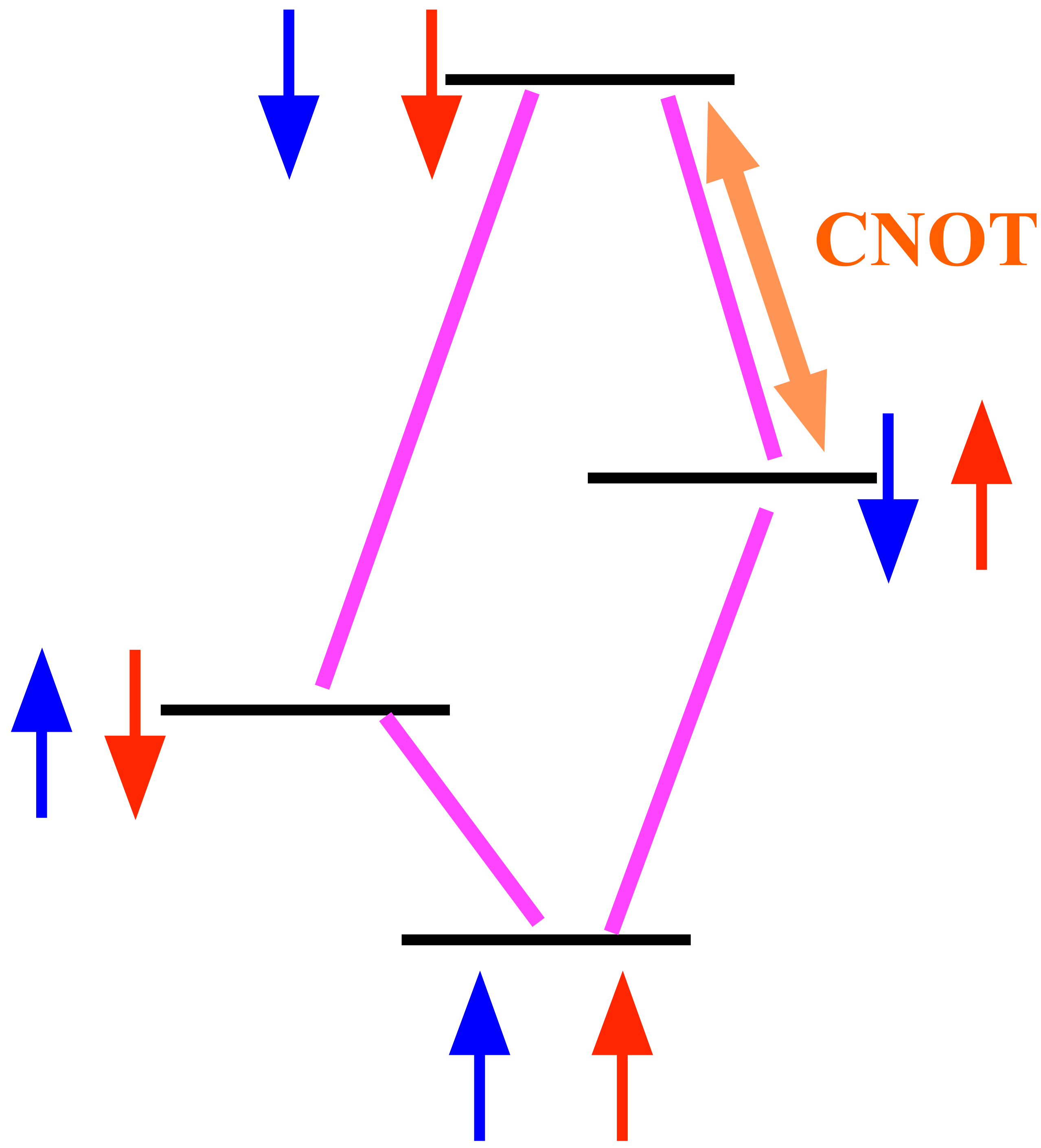
$$\begin{matrix}|00\rangle\\|01\rangle\\|10\rangle\\|11\rangle\end{matrix}\quad\begin{pmatrix}1 & 0 & 0 & 0\\0 & 1 & 0 & 0\\0 & 0 & 0 & 1\\0 & 0 & 1 & 0\end{pmatrix}$$

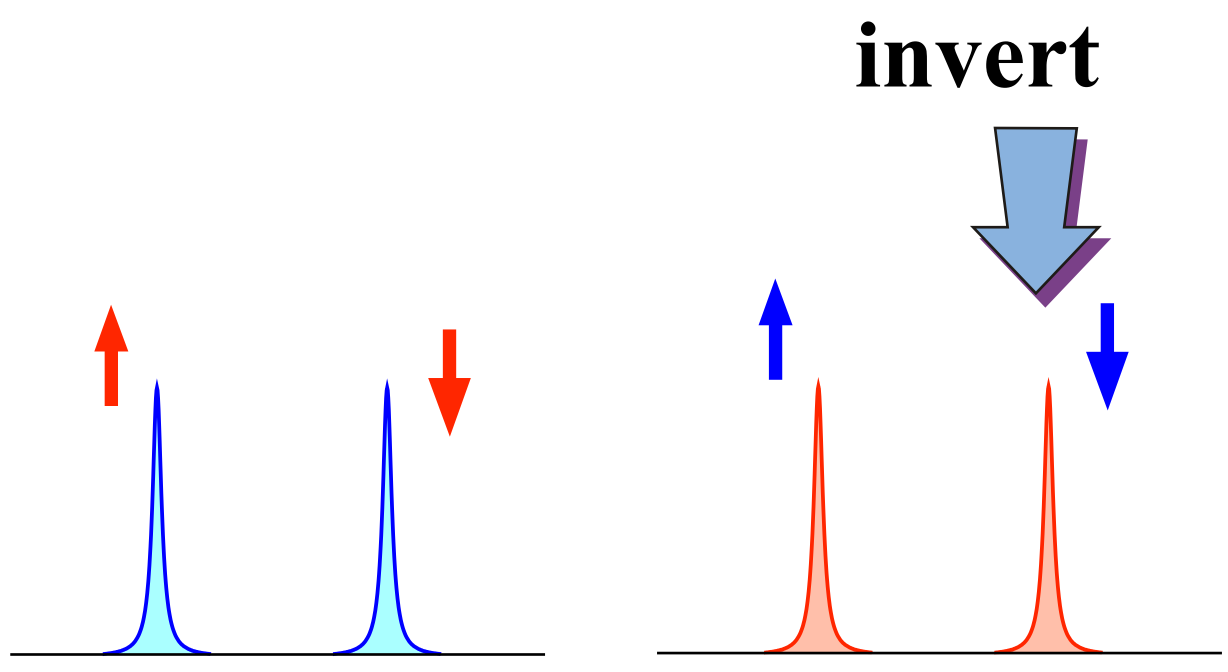


1) Selective Pulses

Example: CNOT

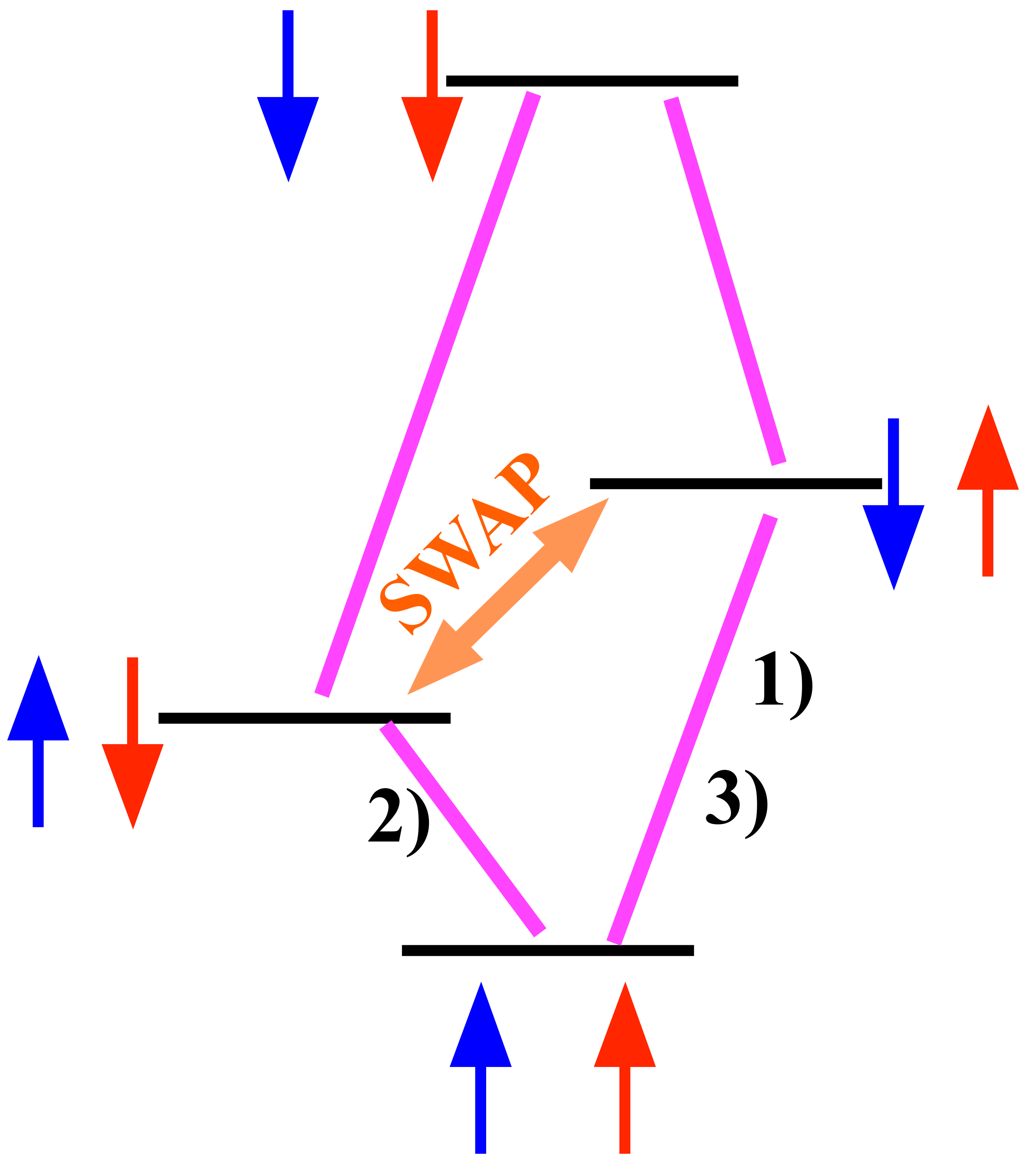
$$
\begin{array}{c} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array}
\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}
$$





1) Selective Pulses

Example: SWAP



1) ↓↑ ⇔ ↑↑

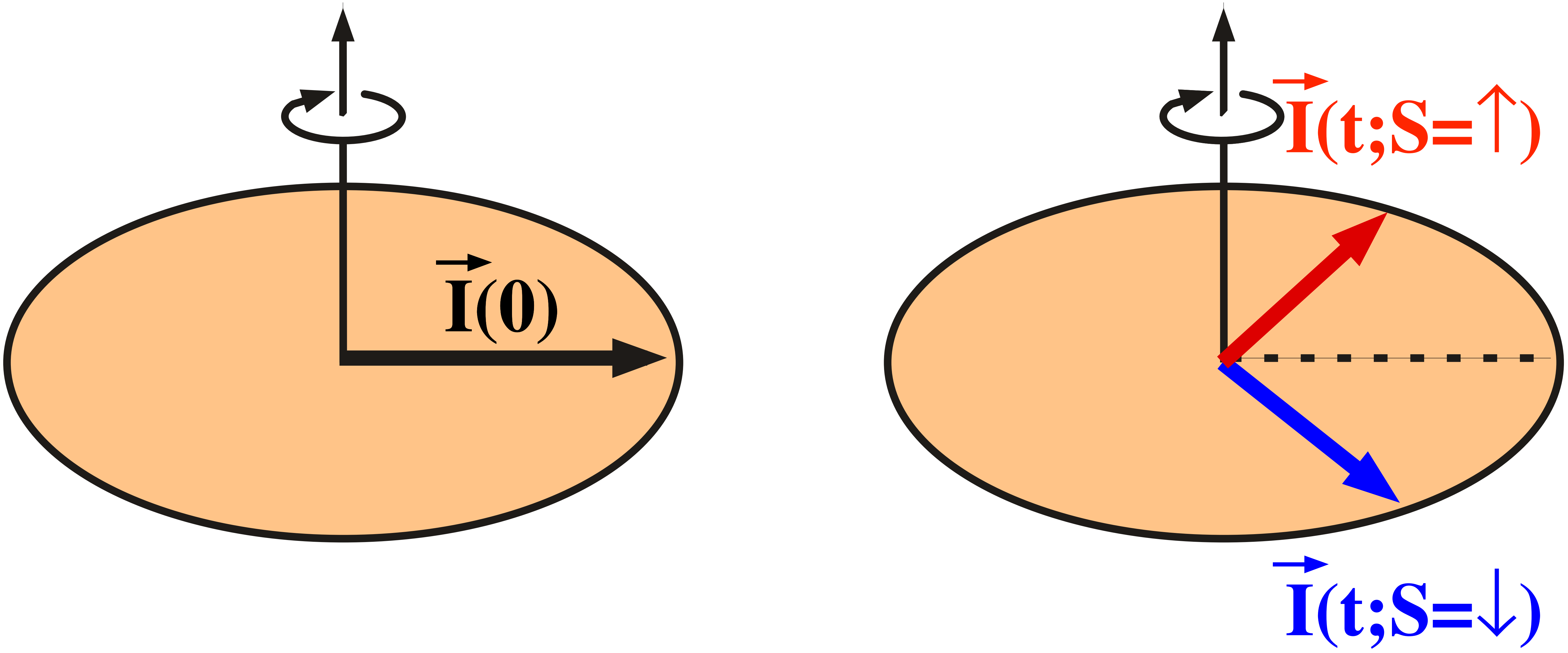
2) ↑↑ ⇔ ↑↓

3) ↓↑ ⇔ ↑↑

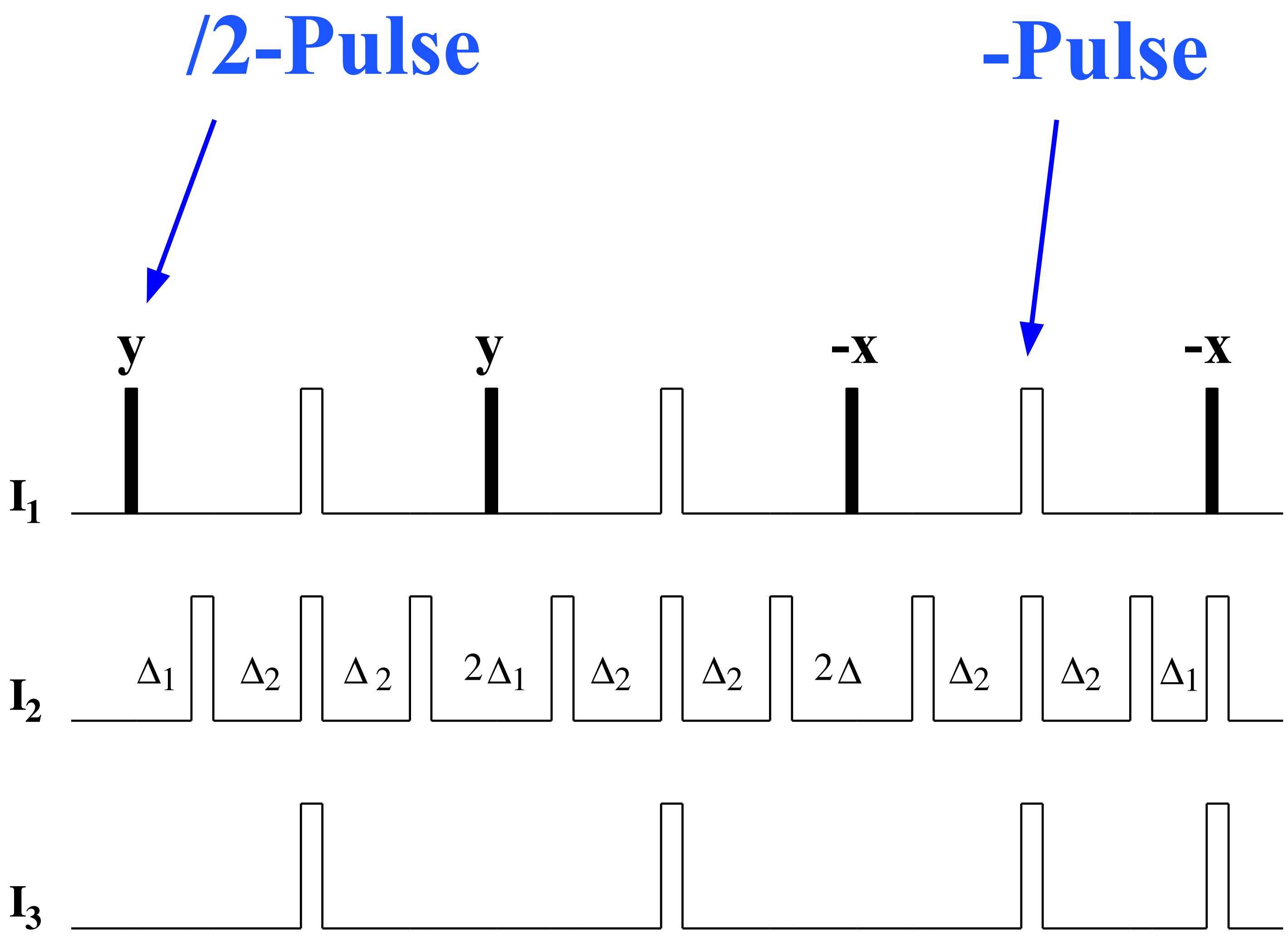
Conditional Dynamics

Spin-Spin Coupling: $\mathbf{H_{IS} = d\, I_z S_z}$

Dynamics of Spin I depends on state of spin S

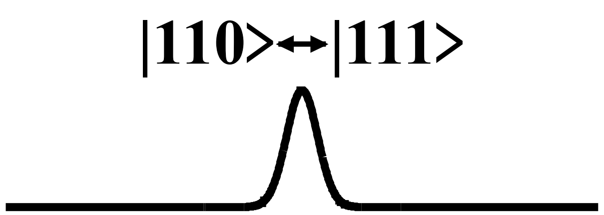


TOFFOLI Gate



Soft pulse

(shaped pulse)



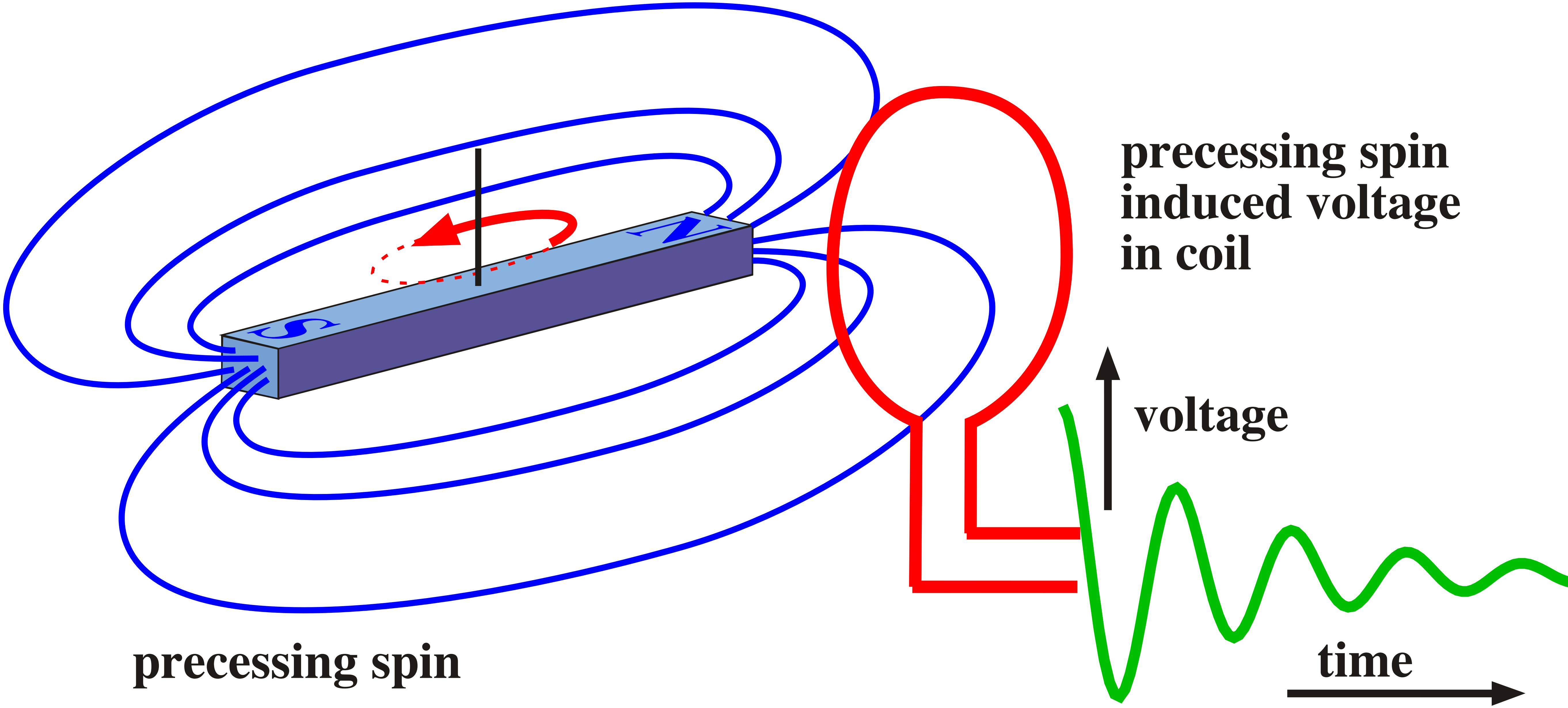
$$\left[\pi_y^{|110\rangle\leftrightarrow|111\rangle}\right] = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Pulses + free precession

Mahesh, PhD thesis (2003).

NMR Detection

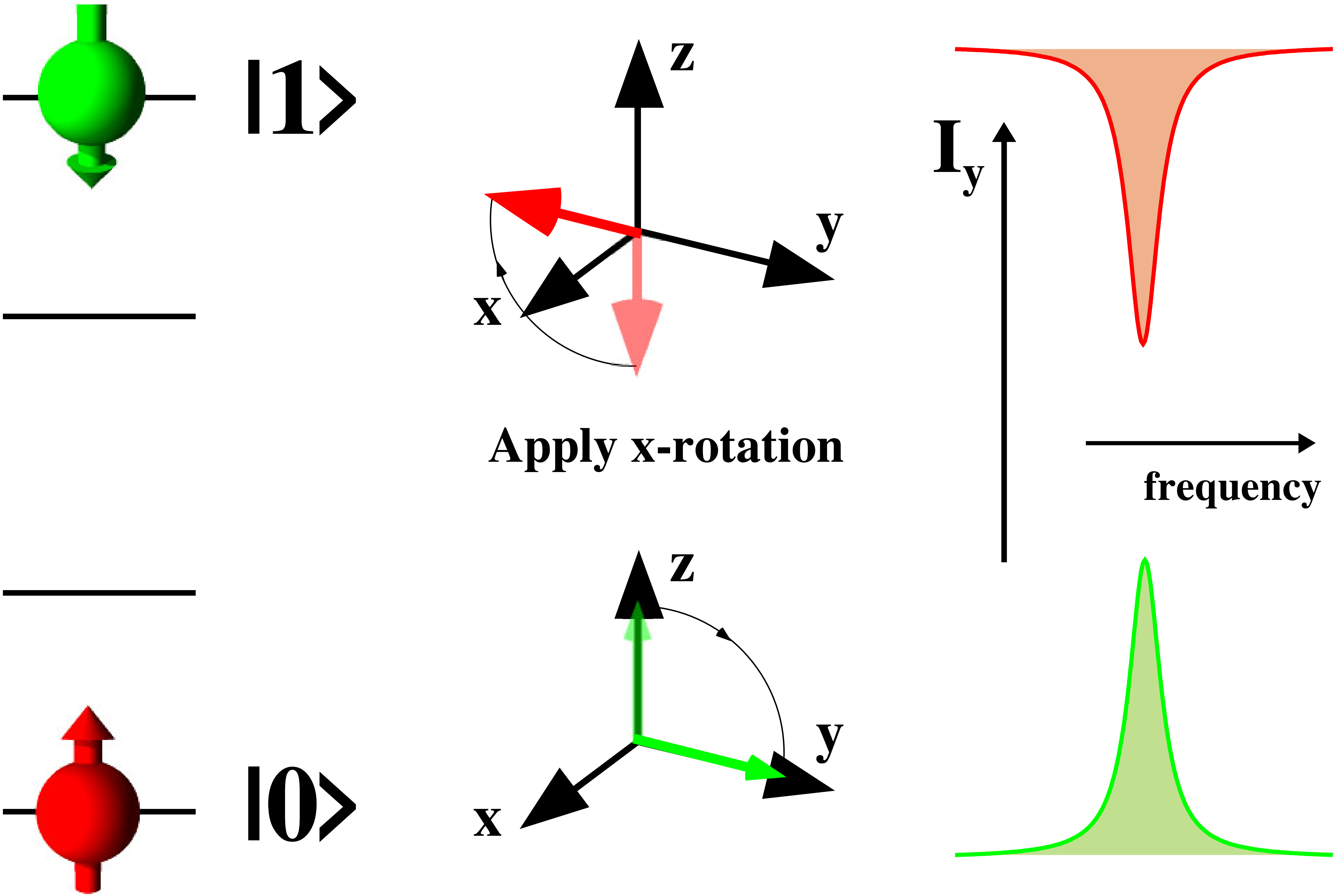
Detection of precessing magnetization by Faraday effect



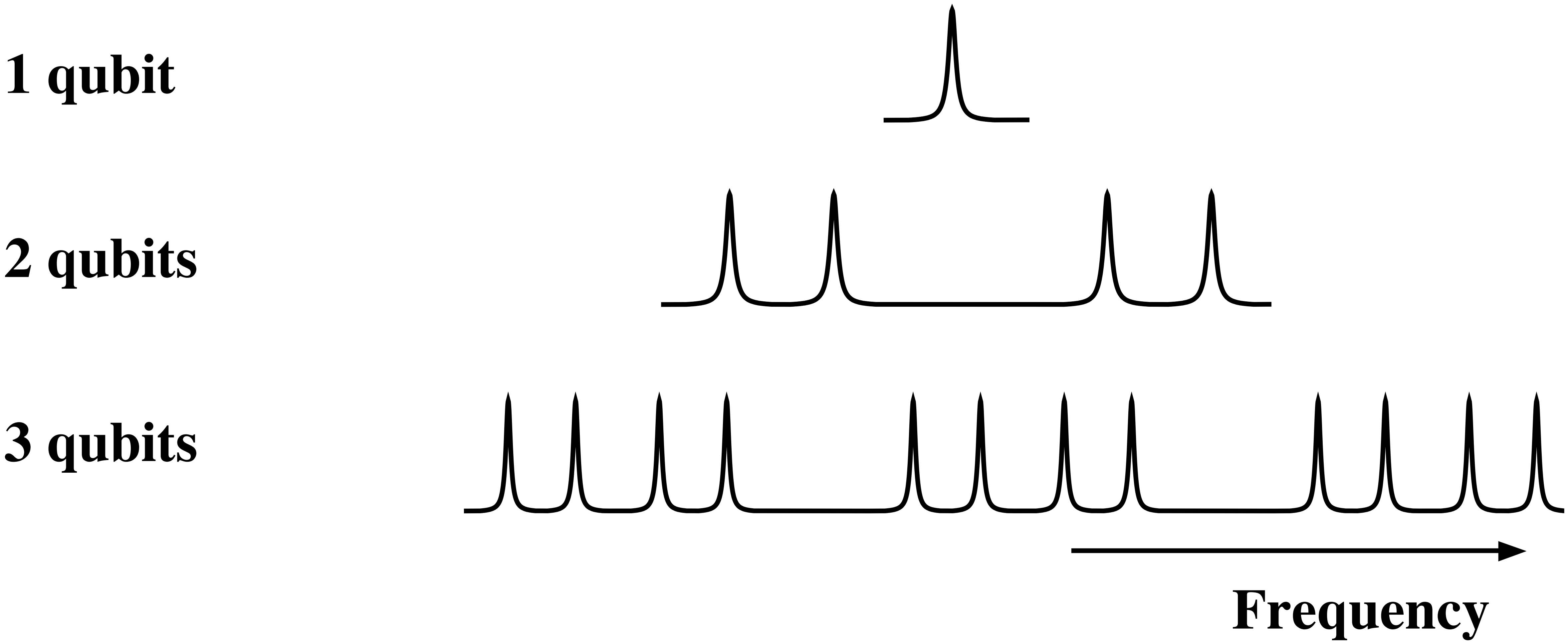
precessing spin
= rotating magnetization

No collapse of wavefunction !

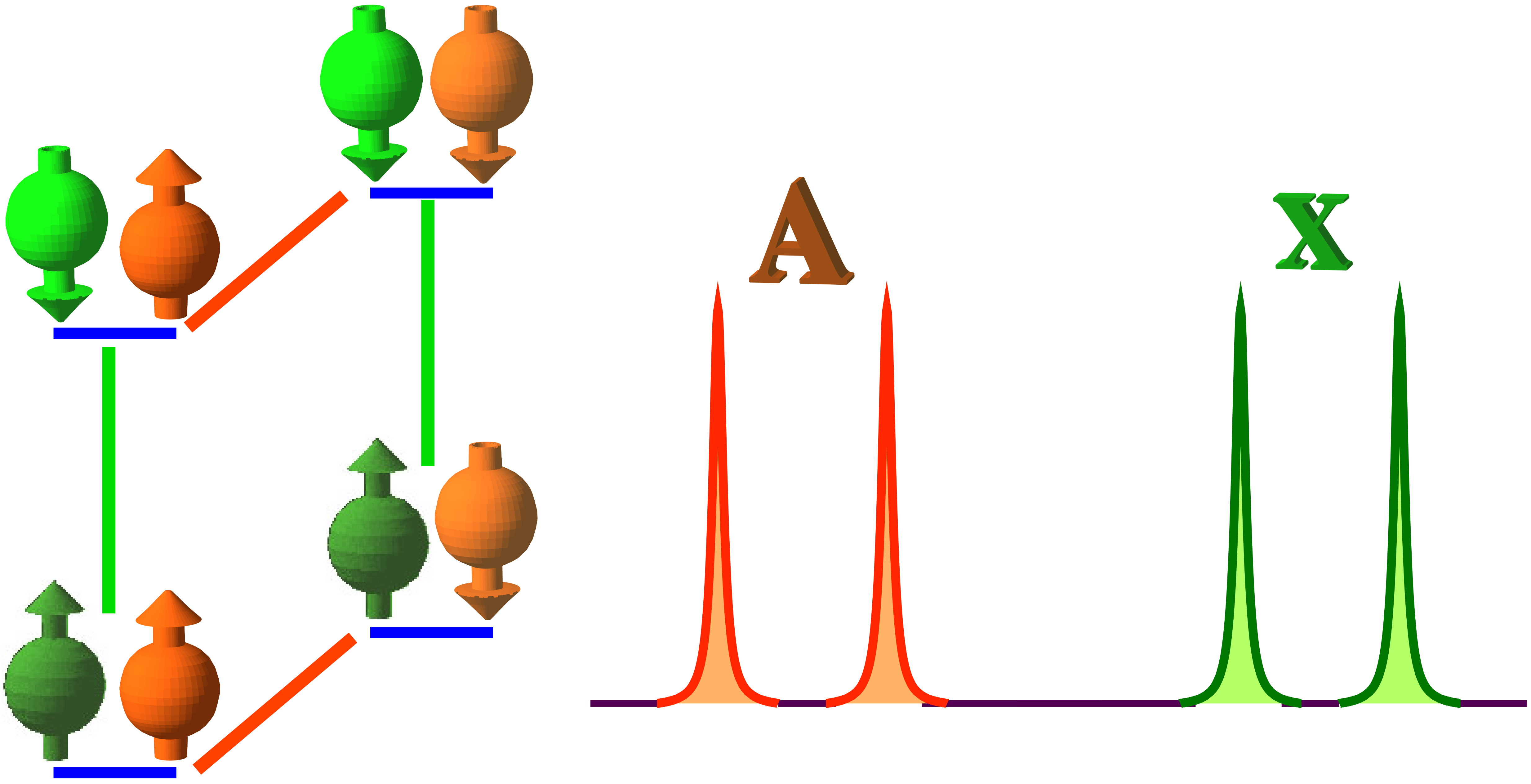
Measuring Populations



Multi-Spin Systems



AX Detection



Qubit-selective Readout

ρ before pulse | A Spectrum (selective pulse) | X Spectrum (selective pulse) | AX Spectrum (nonselective pulse)

A X

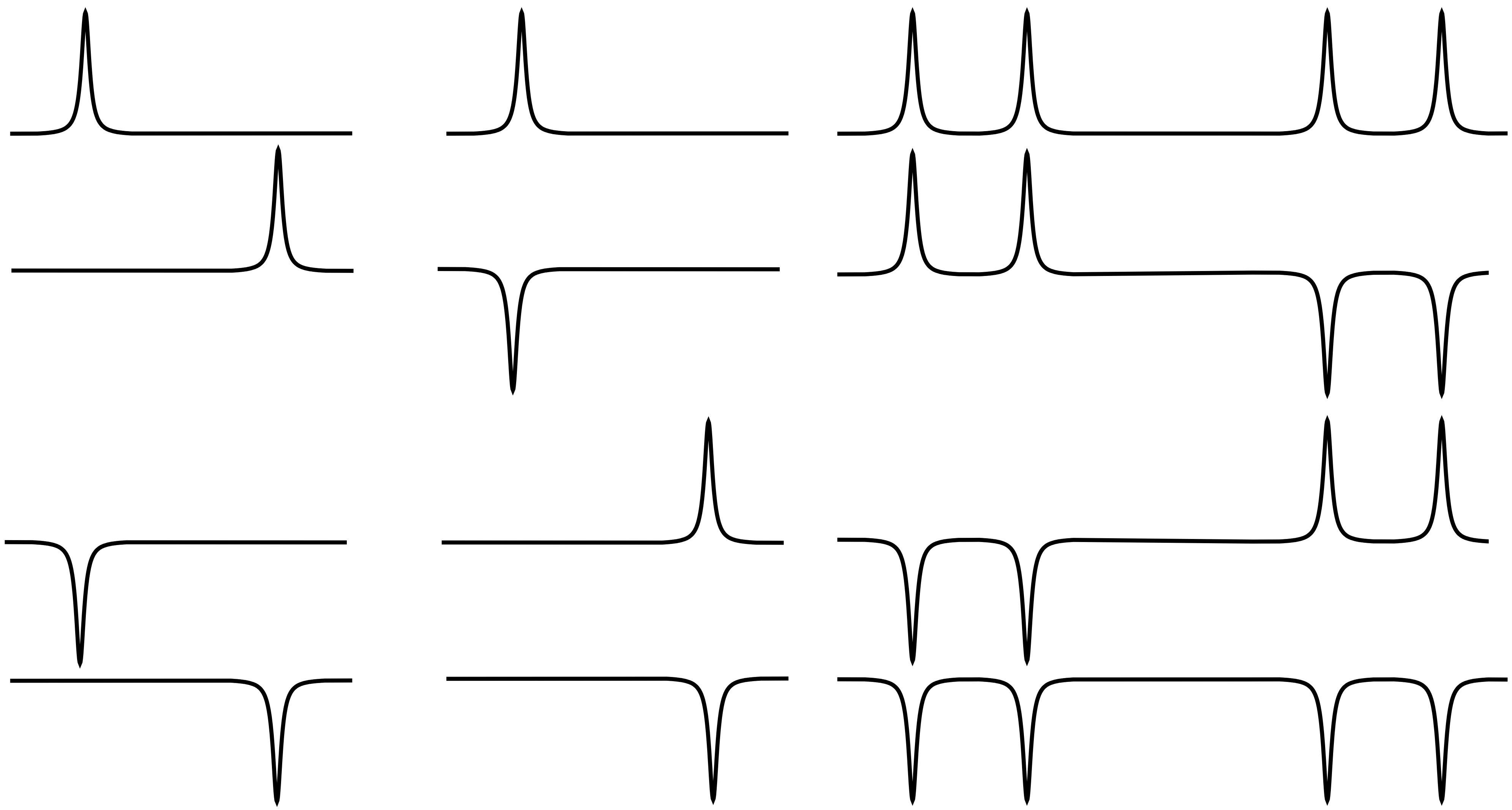
|0> |1> |0> |1> A X

|00>

|01>

|10>

|11>

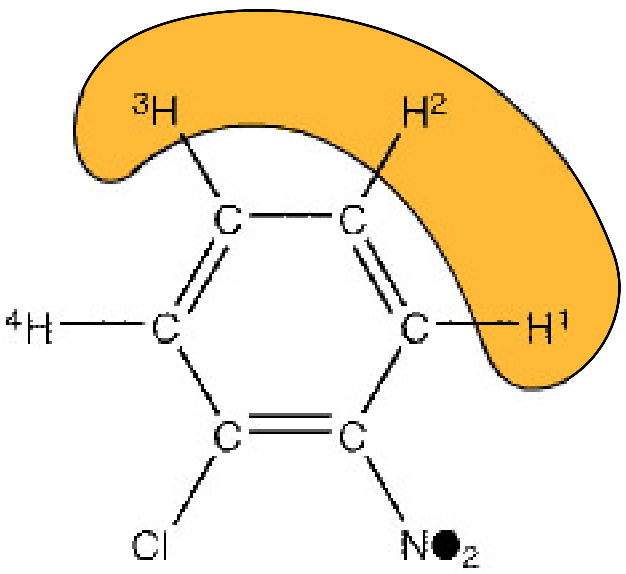


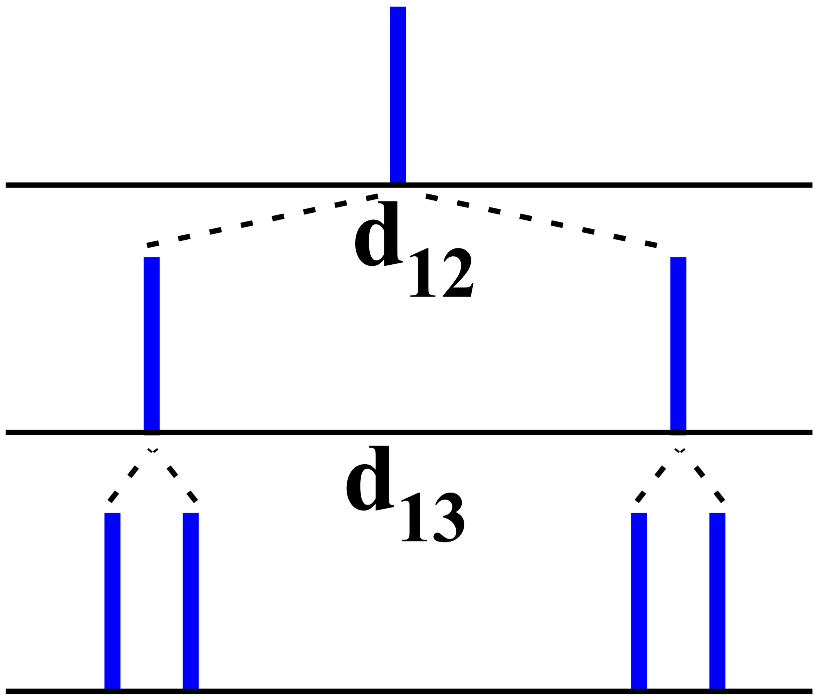
Multi-qubit Readout

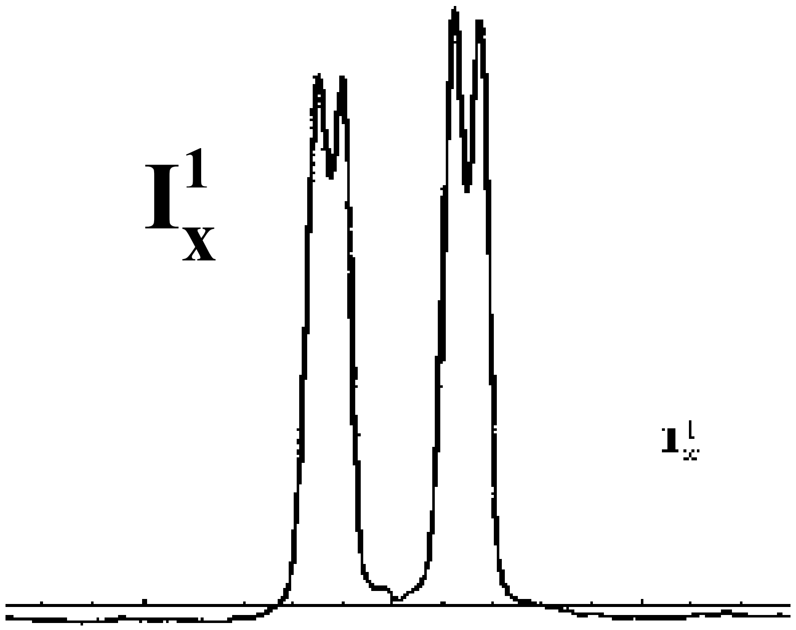
Nuclear magnetic resonance spectroscopy: An experimentally accessible paradigm for quantum computing ?

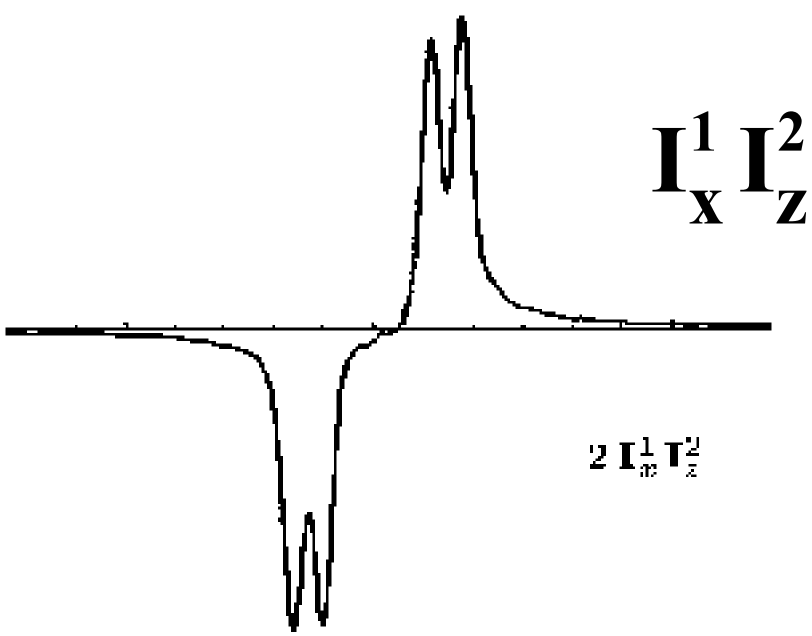
Physica D 120 (1998) 82–101

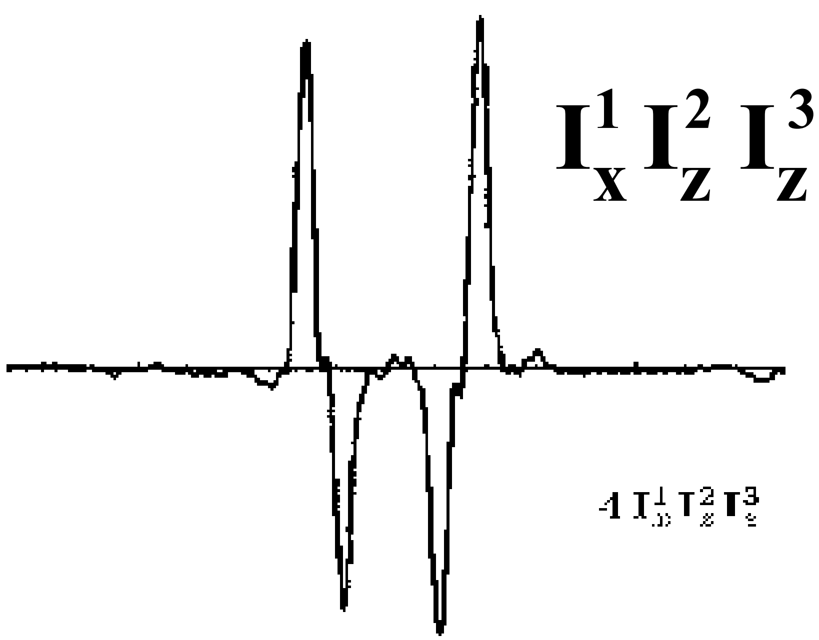
David G. Cory , Mark D. Price , Timothy F. Havel

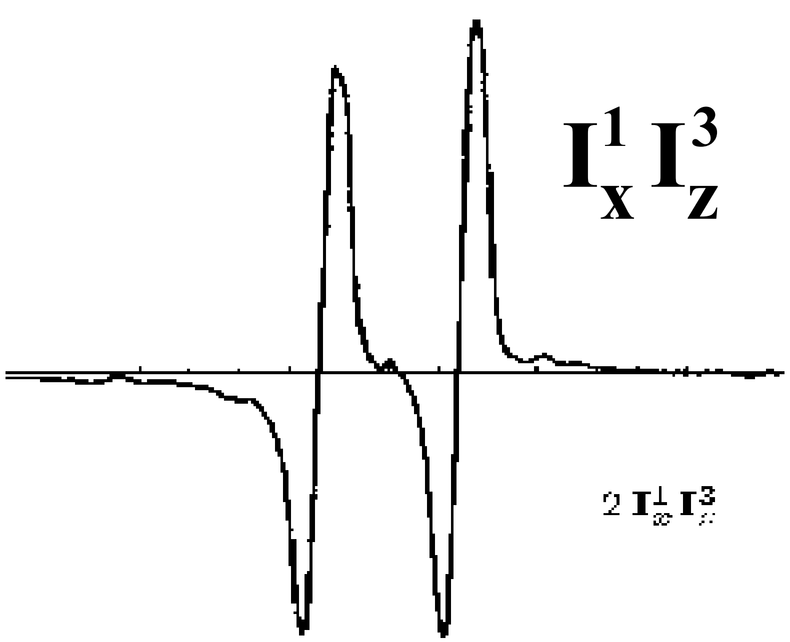








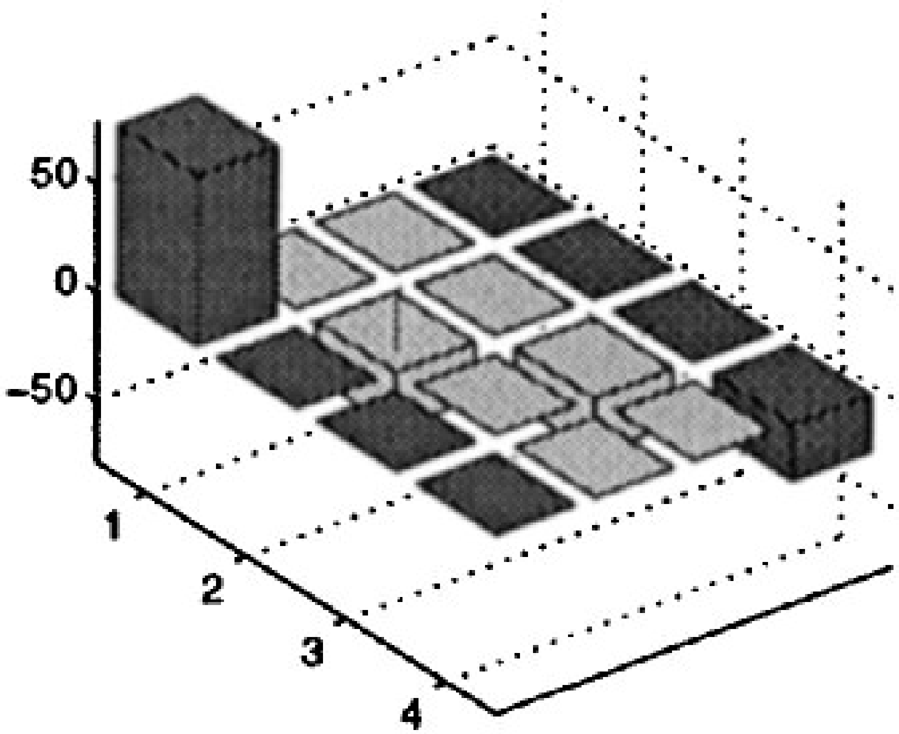


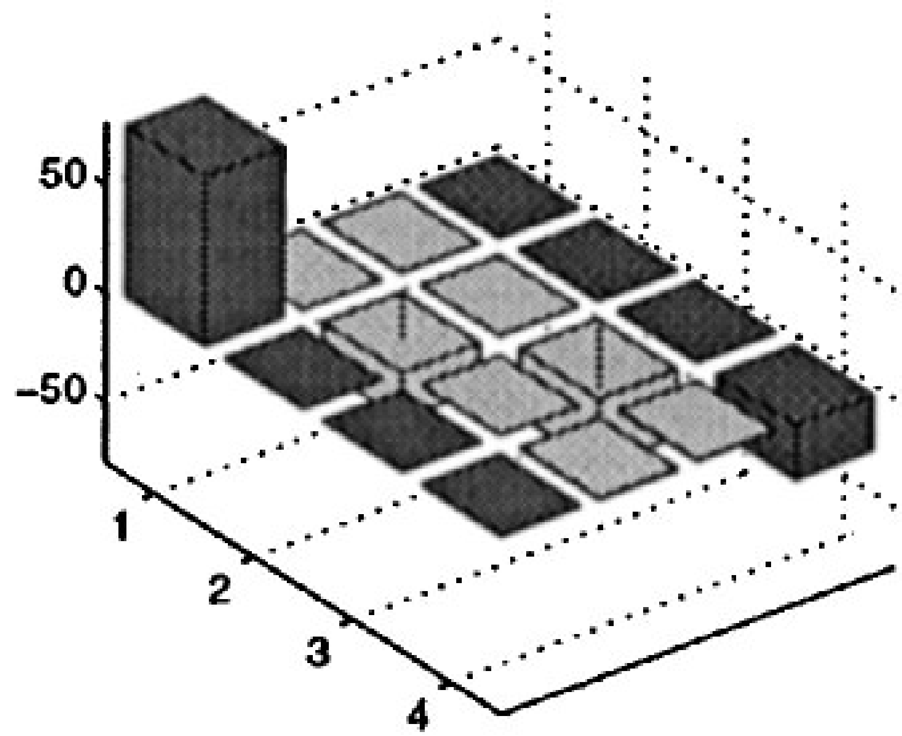


Density Operator Tomography

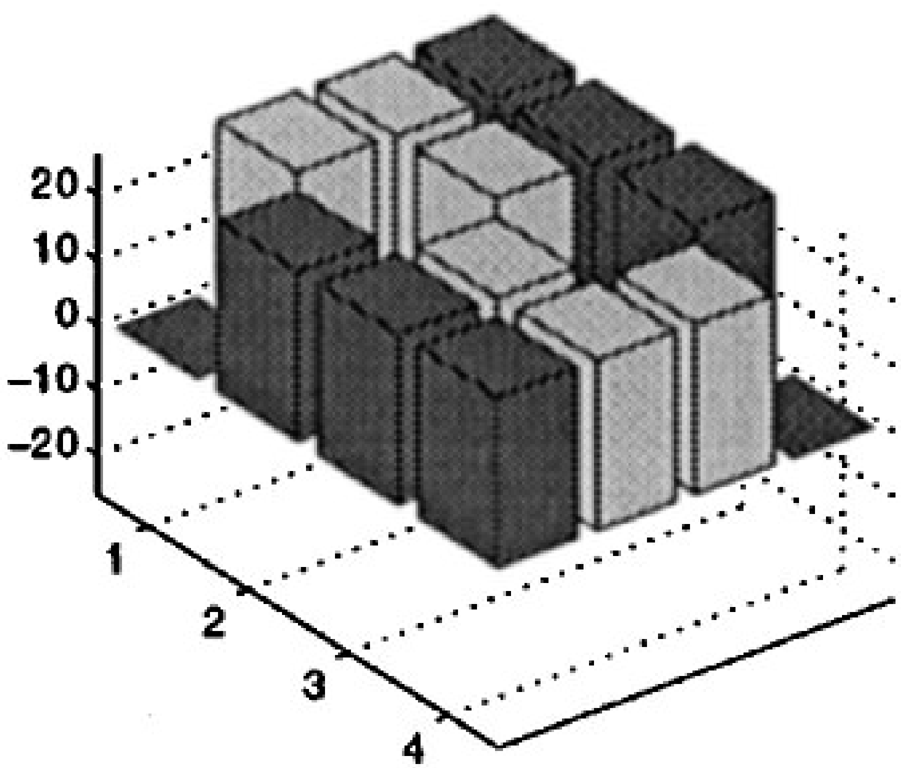
Theory | **Experiment**

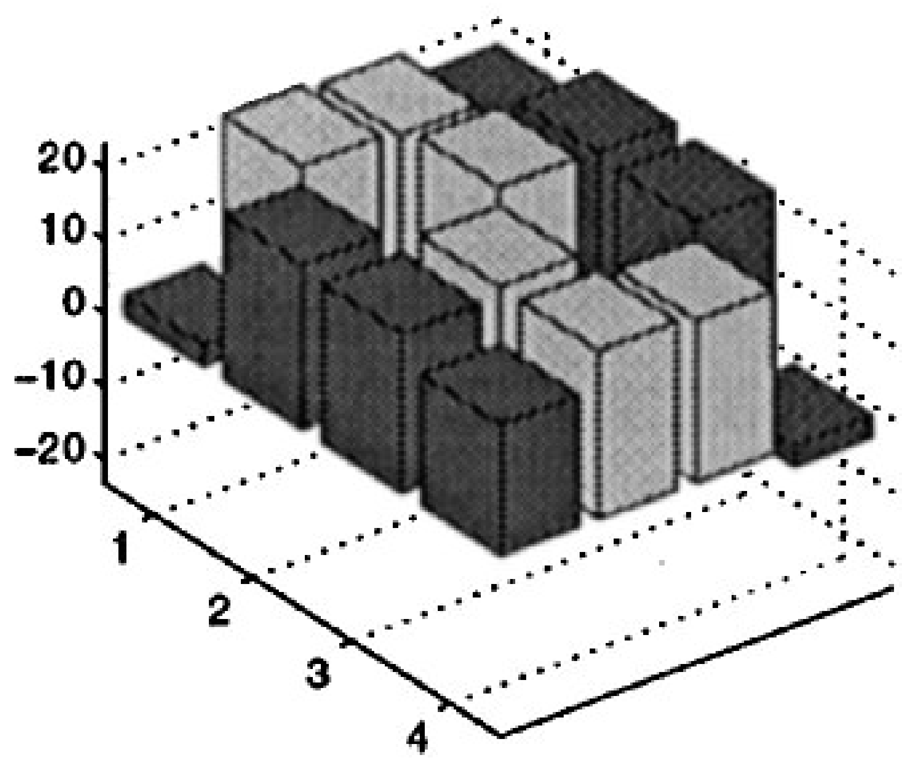
$\rho_{\Delta\,\text{in}}$
0%



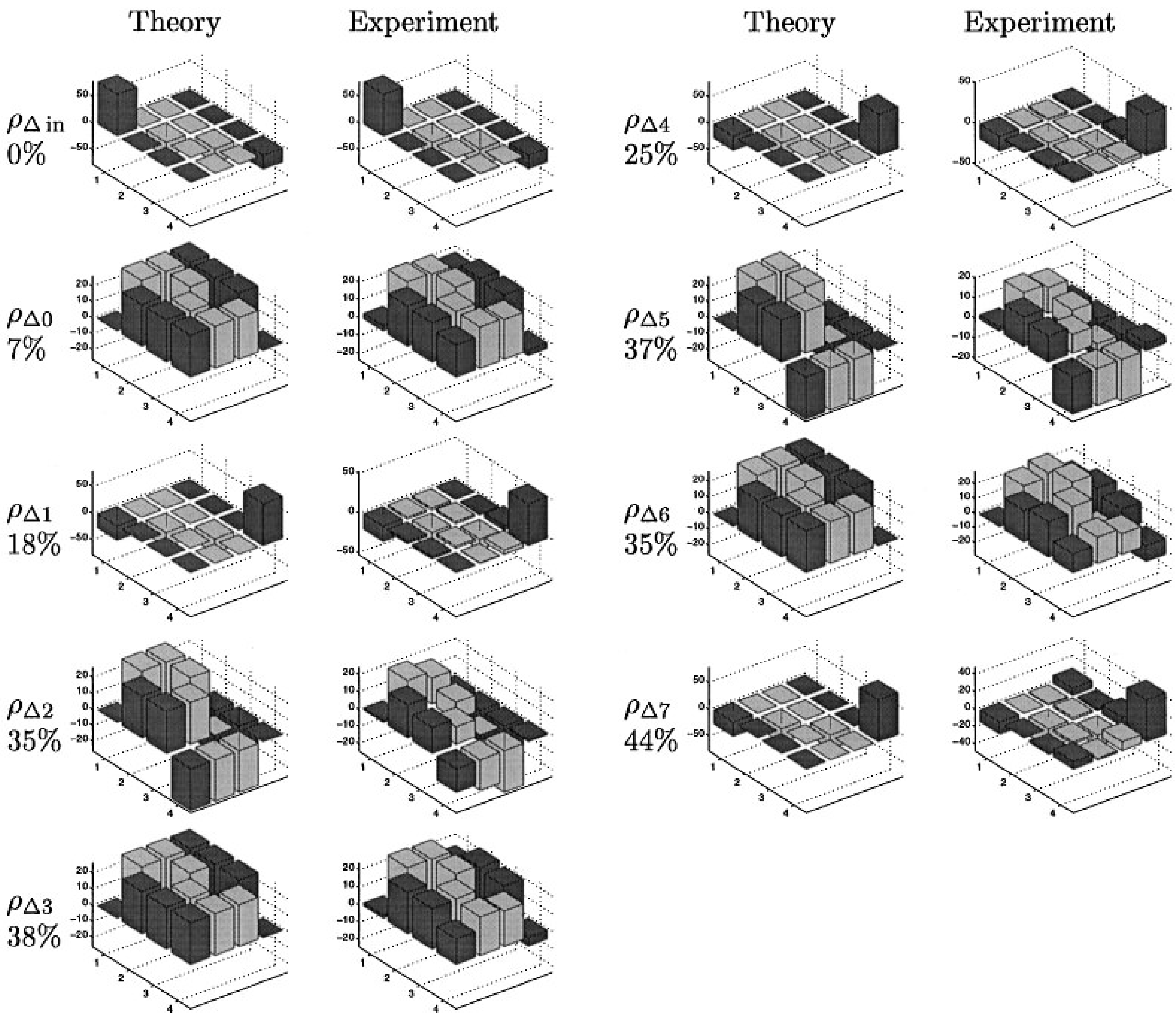


$\rho_{\Delta 0}$
7%

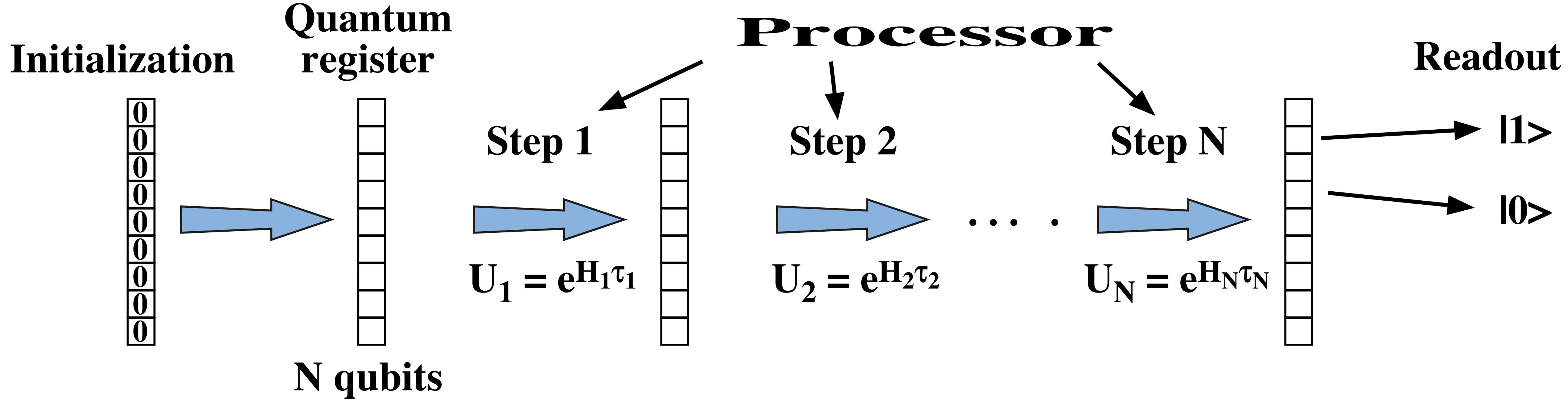




Density Operator Tomography



DiVincenzo's Criteria



1) Well characterized qubits, ~~scalable system~~

2) Initialization into a well defined state.

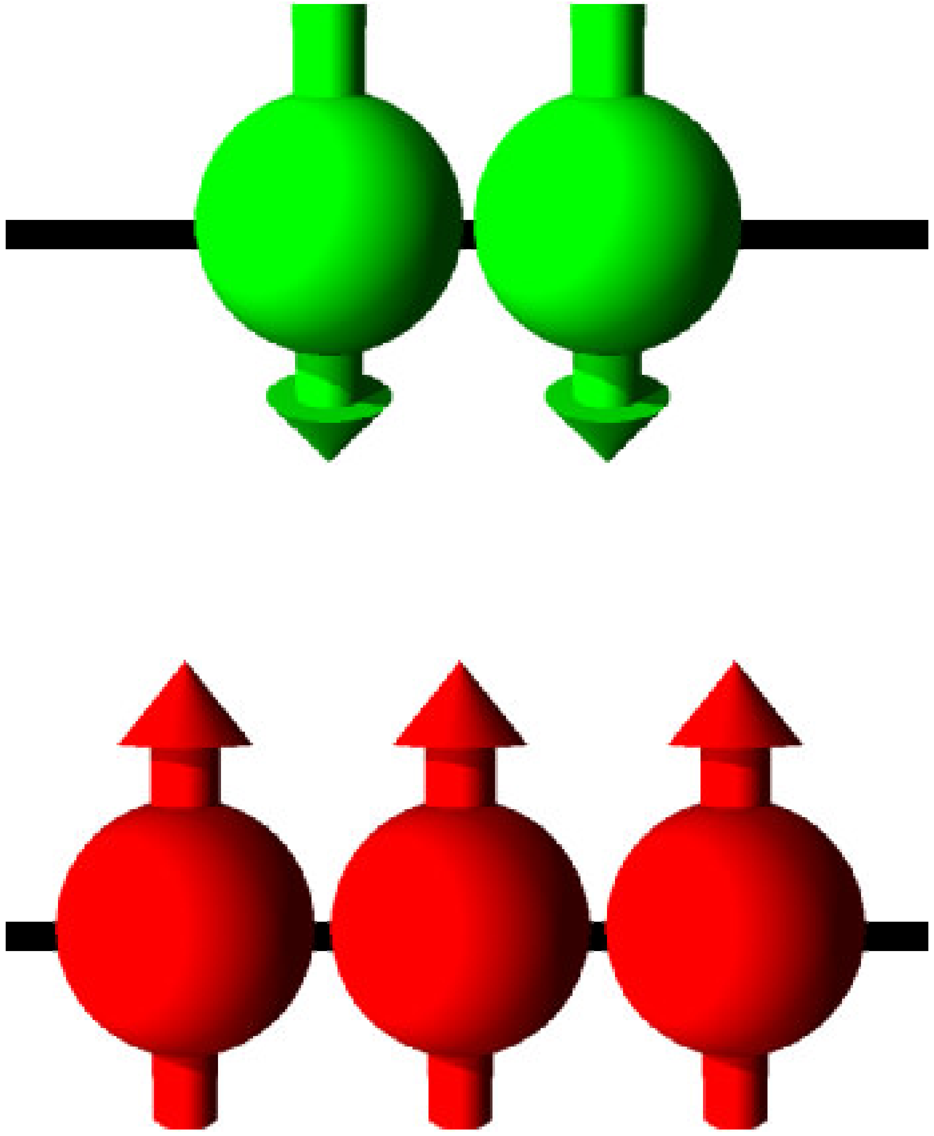
3) Long decoherence times.

4) Universal set of quantum gates.

5) Qubit-selective readout.

DiVincenzo #2 Initialization

Initialization into a well defined state.



Thermal relaxation

$$\rho_{eq} = \mathbb{1} + \varepsilon I_z$$

$\sim 10^{-5}$

Problems:

- not a pure state
- relaxation is slow

DiVincenzo's Criteria

Decoherence

1) Well characterized qubits, scalable system

2) Initialization into a well defined state.

3) Long decoherence times.

4) Universal set of quantum gates.

5) Qubit-selective readout.

Typical relaxation times ~ 1 s in liquid state NMR

Typical gate duration ~ 10 ms

Gates

DiVincenzo's Criteria

1) Well characterized qubits, scalable syste

2) Initialization into a well defined state.

3) Long decoherence times.

4) Universal set of quantum gates.

5) Qubit-selective readout.

gate = unitary transformation $$U = e^{iHt}$$

Readout

DiVincenzo's Criteria

1) Well characterized qubits, scalable system

2) Initialization into a well defined state.

3) Long decoherence times.

4) Universal set of quantum gates.

5) Qubit-selective readout.