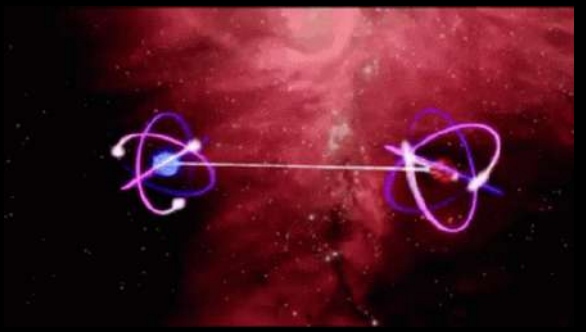
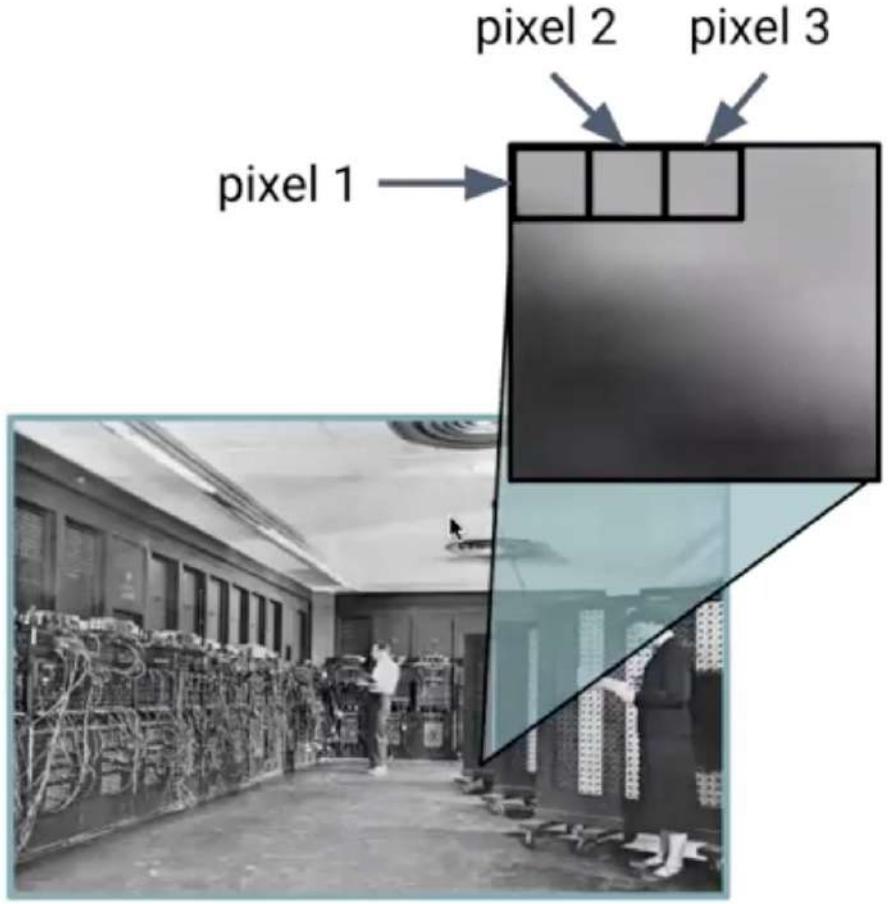
Molecular Spin Qubit for future Quantum Technology

Asif Equbal
Chemistry, NYUAD

Hello, Binary world!!



Example: Mapping a photograph into binaries



Divide the image into pixels

The **brightness** of each pixel is represented by a string of **bits** (e.g. 8 bits)

- 00000000 → Completely dark (Black)
- 11111111 → Completely bright (white)
- 00001111 → in between (gray)

Computational Stacks

NETFLIX

Applications

Gates

Classical Bits

Classical bits are pulses of electricity.

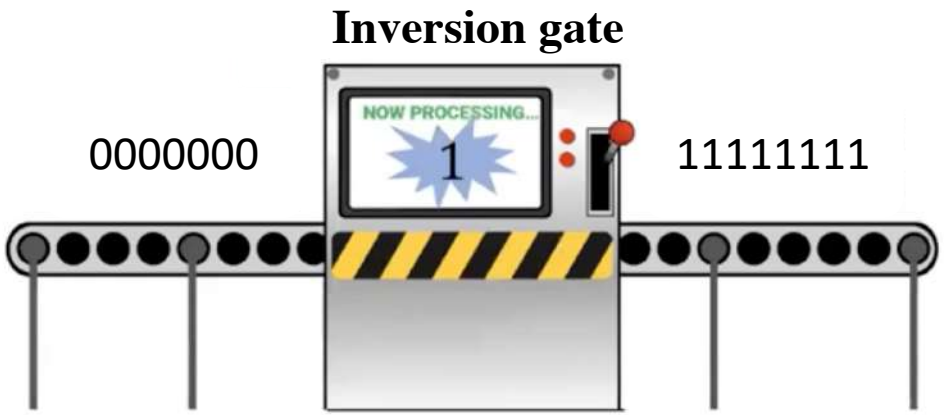
We represent them as 1's and 0's, but physically, they are the presence or absence of electricity.

This is why bits are binary: the electrical pulse is either present or absent. There is no "in-between!"

Gates: Manipulate bits

Takes Inputs (0 1 1 0 0 1 …..) and Spits Outputs (1 0 1 1 0 0 …….)

Example: Invert color map of an image



Computational Stacks

NETFLIX

Applications
A combination of algorithms

Algorithms
A combination of circuits

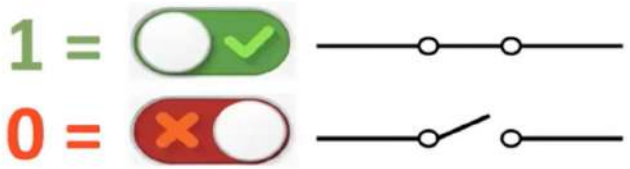
Circuits
A combination of gates

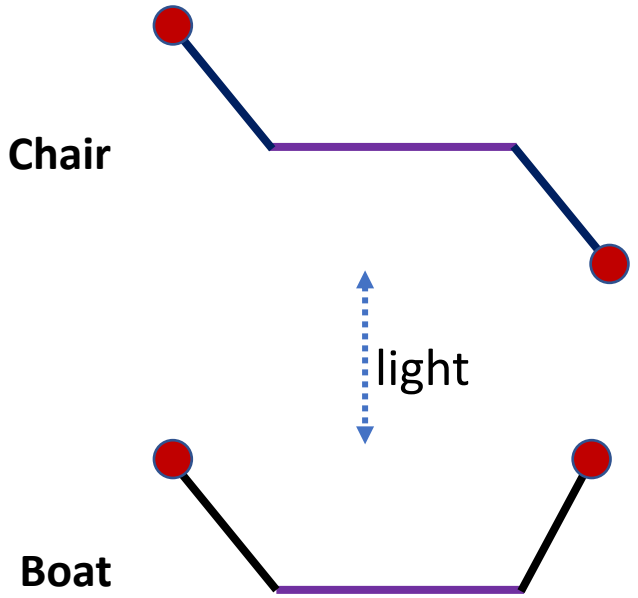
Gates
Operate on Bits

Classical Bits
Basic information storage unit

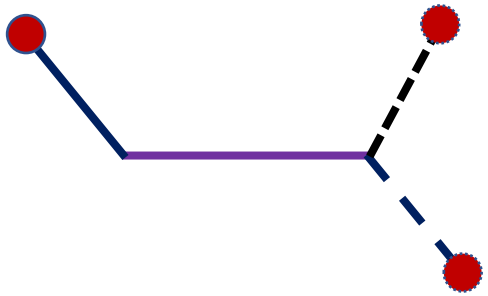
Classical Bits → Quantum Bits (qubits)

Classical





Quantum

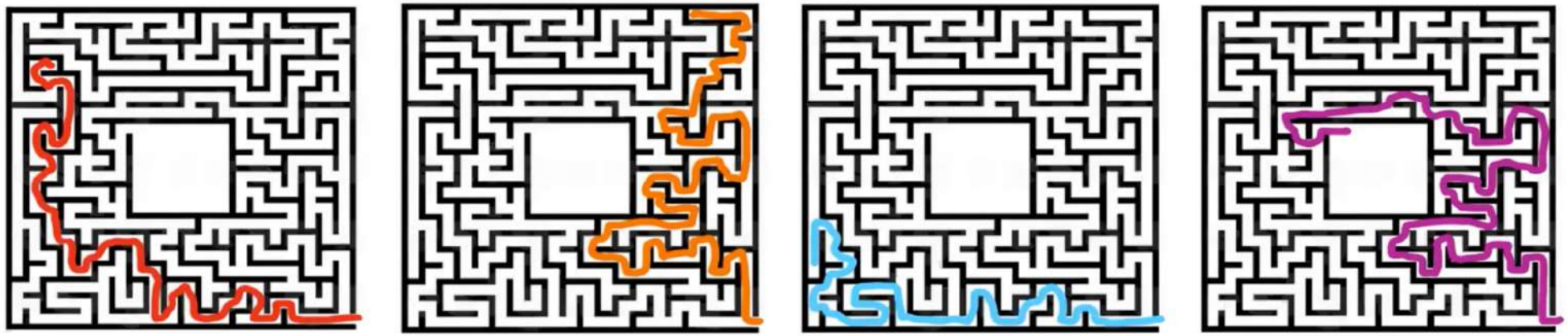


Chair + Boat

Superposition!

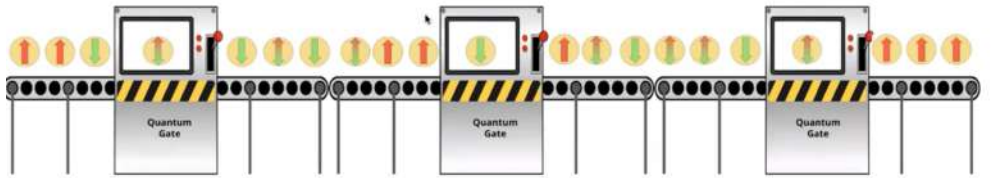
Quantum Advantage

Classical



Quantum

A quantum circuit is a sequence of **quantum gates.**



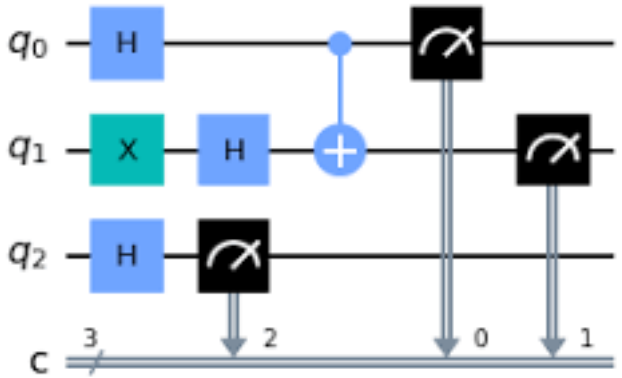
Quantum Computation

1981: Idea of Quantum

1994: Shor's Algorithm

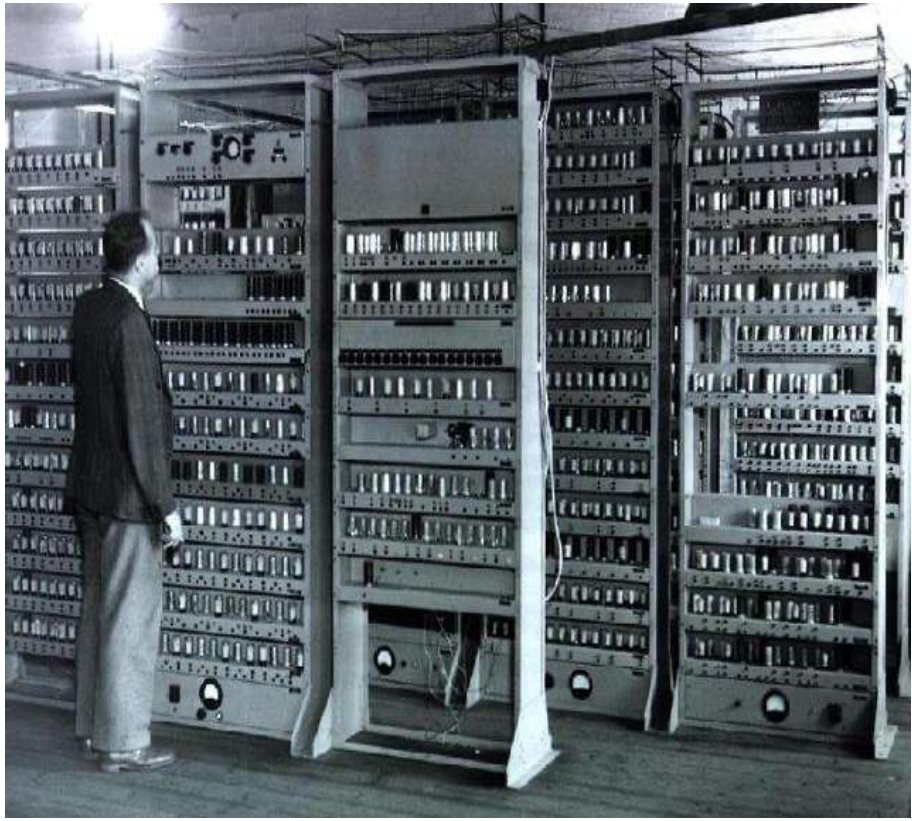
1998: Experimental Quantum algorithm demonstration

2019: Quantum Advantage Achieved by Google



Current State of Quantum Computers… ?

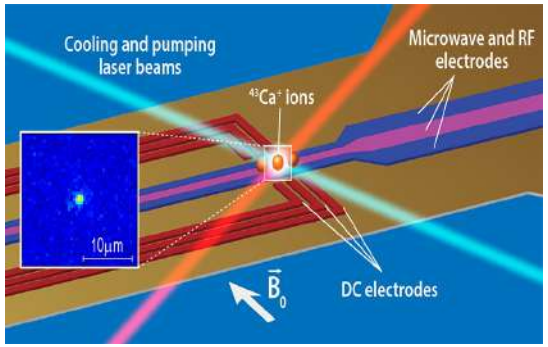
under construction….

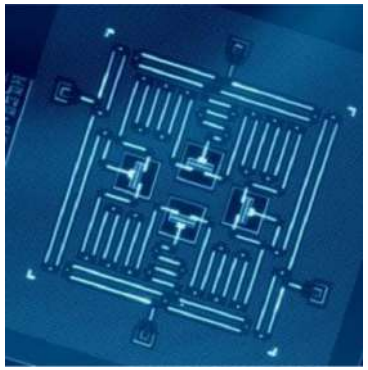


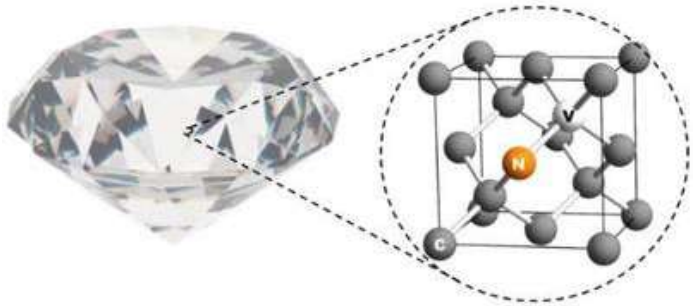
Old Classical Computers

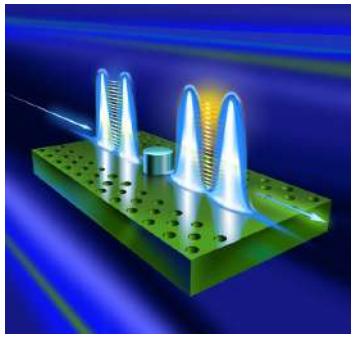
Current Quantum Computers

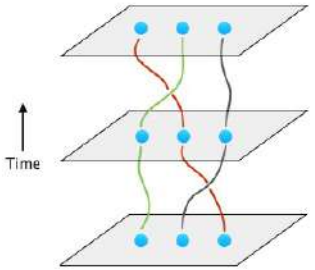
Quest for the “ideal” Qubit!











- IonQ
- Google
- IBM
- Intel
- Academic Labs
- Microsoft

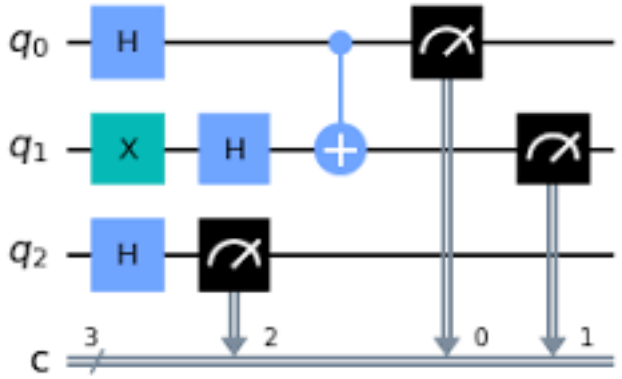
It’s not clear what the best Qubit maybe!

Different Qubit system requires different processing approach (gates) → Different Quantum Computers

DiVencizio's criteria

❖ 5 minimal requirements he predicted were necessary for creating a **quantum** computer

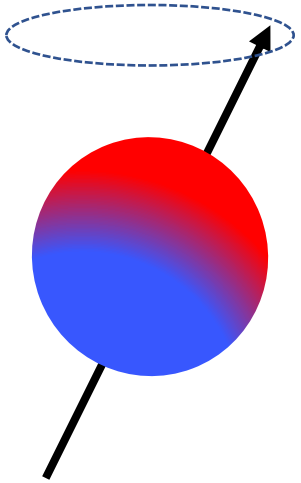
1. Scalable
2. Initialization
3. Universal set of quantum gates
4. Long decoherence times
5. Qubit-specific measurement



❑ Developed **Spin** based Quantum Computer !!

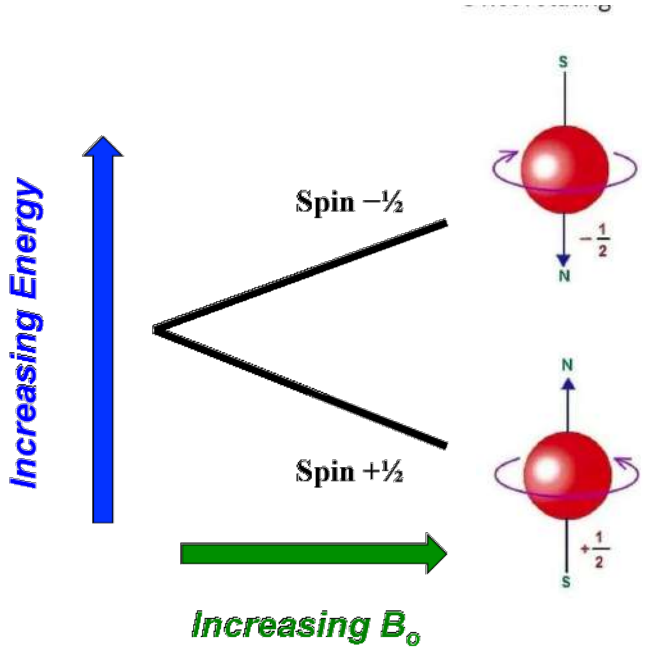
Spin ??

Precession; $\boldsymbol{\omega} \propto \boldsymbol{\gamma}$ B



Spin: Imagine a ball that's rotating,
except it's not a ball and it's not rotating.

Zeeman Effect:



1

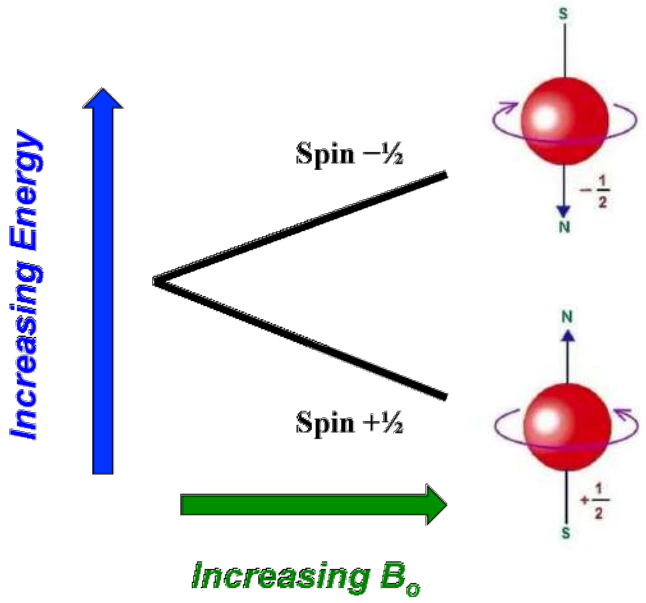
0

Spin Qubit

Zeeman effect: Spin-Magnetic field interaction

Spin: nuclei of atoms *(1H, 13C, 19F, 31P),* electrons, photons

Zeeman Effect: $\mathbf{H_{zeeman}} = -\boldsymbol{\mu}.\boldsymbol{B} = \omega\, I_z$



$$\hat{H}_{Zeemann}\,|\mathrm{I}, m\rangle = -\gamma B_0 I_z\,|\mathrm{I}, m\rangle = -\omega_0 I_z\,|\mathrm{I}, m\rangle$$

$\|1/2\rangle$	$\|-1/2\rangle$
$\omega_o/2$	
	$-\omega_o/2$

Spin -1/2

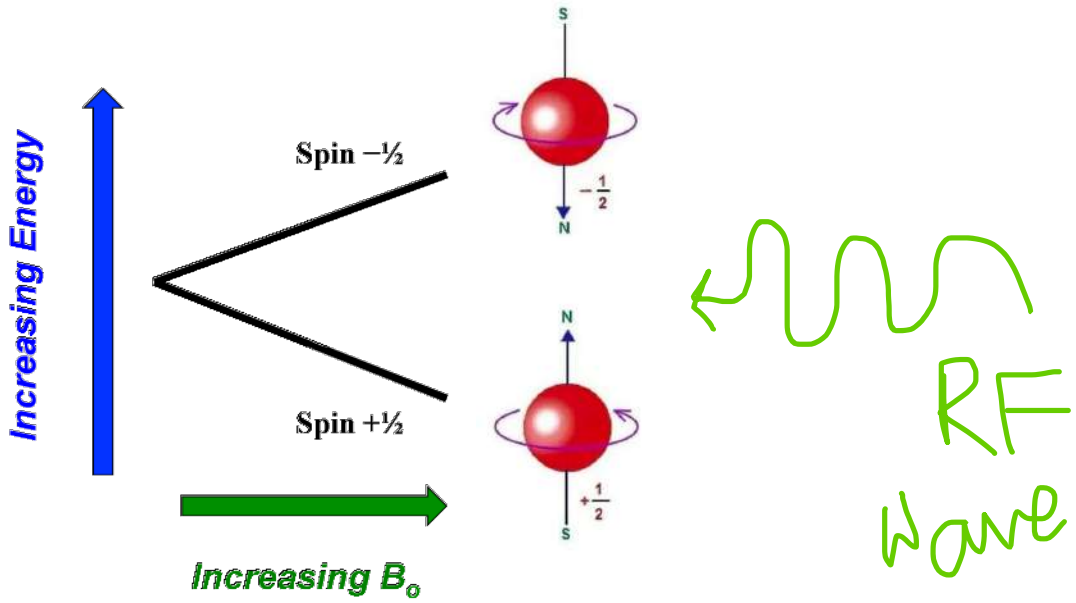
Radio Frequency Interaction: Manipulate Spin-states

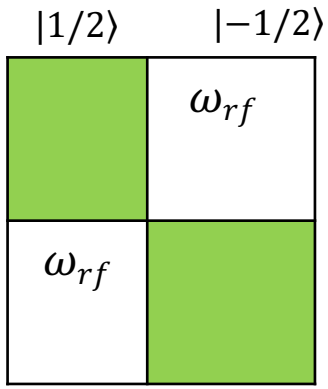
RF: Oscillating magnetic Field; Resonance

$$H_{rf} = \omega_{rf}[I_x \cos(\omega_0 t + \phi) + I_y \sin(\omega_0 t + \phi)] + \omega_{rf}[I_x \cos(-\omega_0 t + \phi) + I_y \sin(-\omega_0 t + \phi)]$$

$$H'_{rf} = e^{i\omega_0 I_z t} H_{rf} e^{-i\omega_0 I_z t}$$

$$H_{rf}(rotating frame) = \omega_{rf}[I_x \cos(\phi) + I_y \sin(\phi)]$$



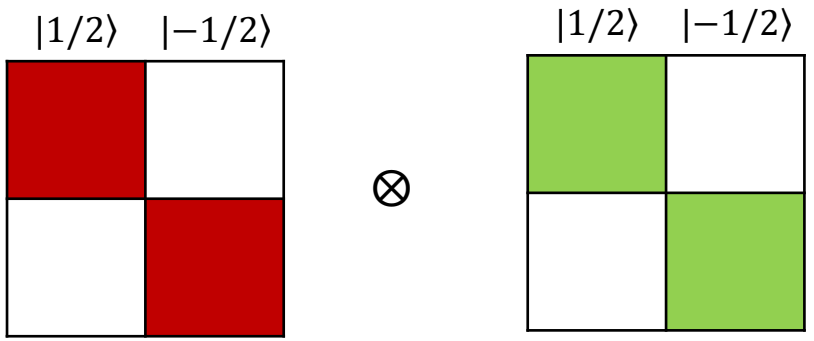


Spin -1/2

Single-qubit gate (e.g. X-gate, H-gate)

Coupling Interaction: Spins-entanglement

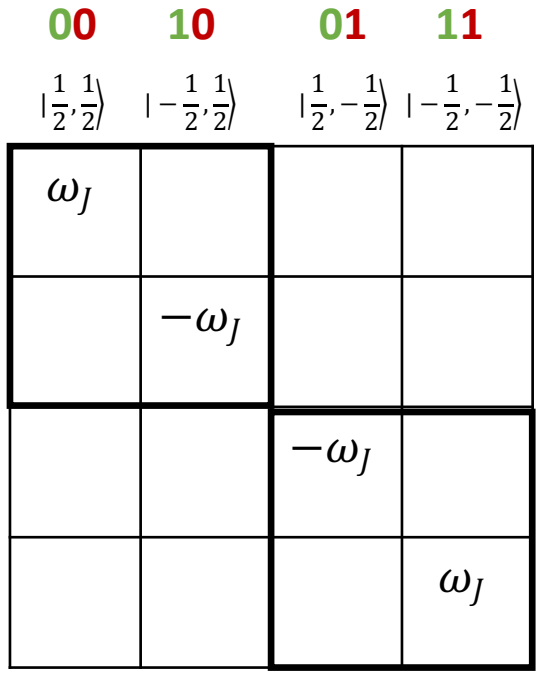
$$\mathbf{H_{coupling}} = 4.\,\omega_j\, I_z\, S_z$$



Spin - I **Spin - S**

Qubit-0 **Qubit-1**

Product basis



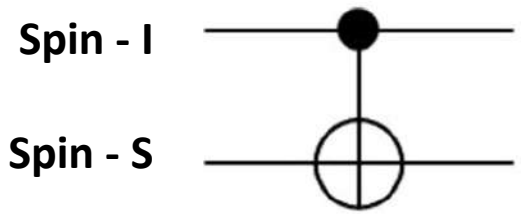
Spin 1/2 + Spin 1/2

Coupling Interaction: Spins-entanglement

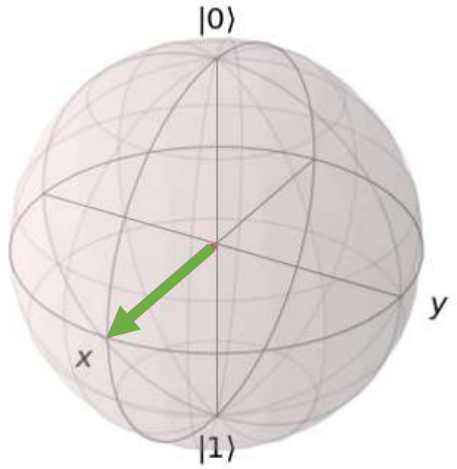
$$\mathbf{H_{coupling}} = 4.\omega_j \, I_z \, S_z$$

00	10	01	11
$\left\|\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\|-\frac{1}{2},\frac{1}{2}\right\rangle$	$\left\|\frac{1}{2},-\frac{1}{2}\right\rangle$	$\left\|-\frac{1}{2},-\frac{1}{2}\right\rangle$
ω_J			
	$-\omega_J$		
		$-\omega_J$	
			ω_J

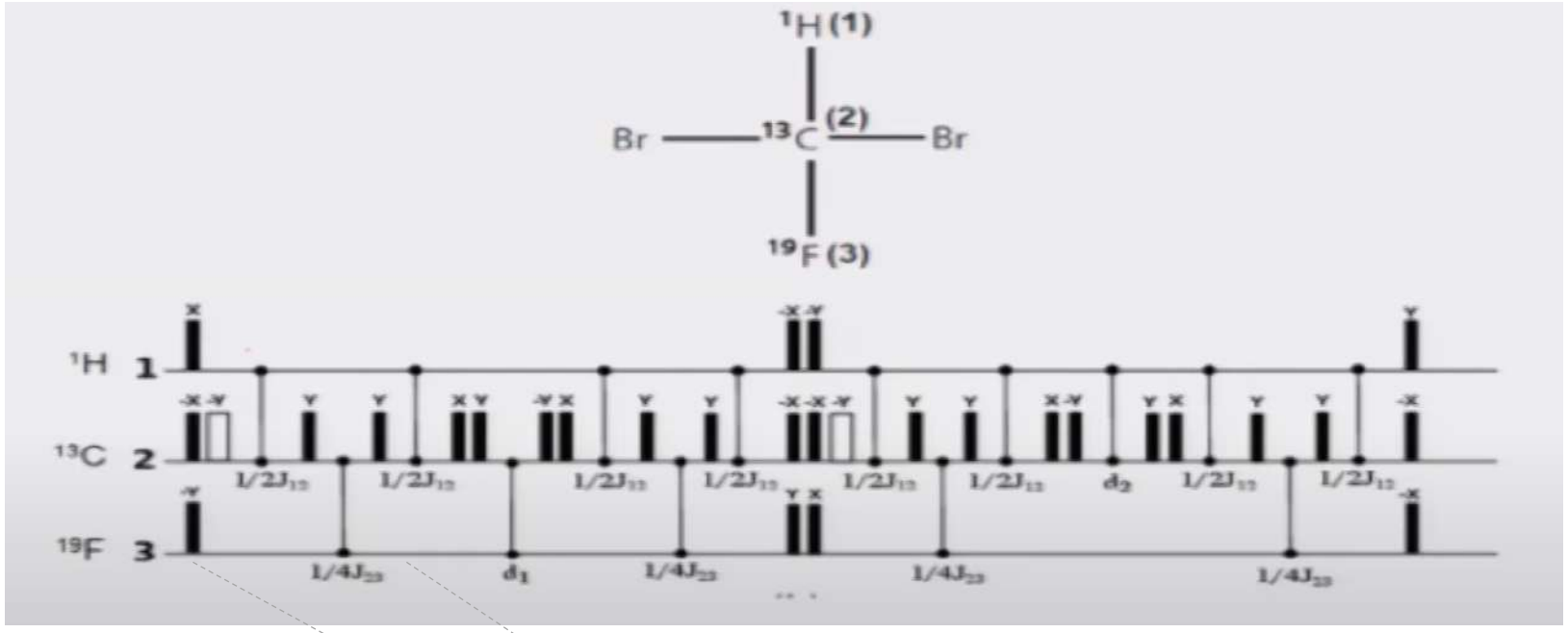
Spin 1/2 + Spin 1/2



$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



NMR Quantum Computer

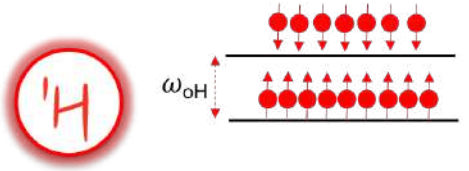


Unitary operators

- ✓ Universial quantum gates
- ✓ Grover's search algorithm
- ✓ Quantum fourier transform
- ✓ Shor's algorithm
- ✓ DJ algorithm

Problem with NMR Quantum Computer

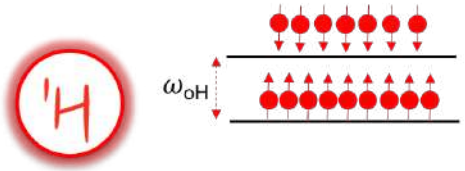
1. Molecular Stability, Felxibity → Scalable
2. Low polarization → Initialization is an issue → Only Pseudo-initialization possible
3. Slow Relaxation → Long decoherence times
4. Coupled system → Universal
5. Heteronuclear → Specific measurement



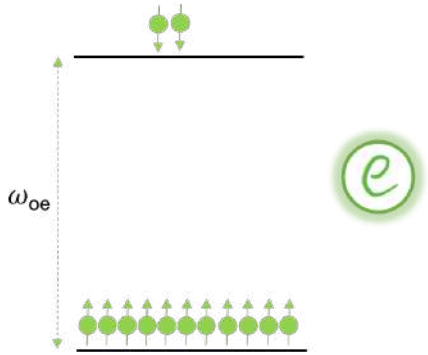
- Almmost equal population in two sub-levels!

Search for well-initialized Qubit

❖ **Poor Initialization**

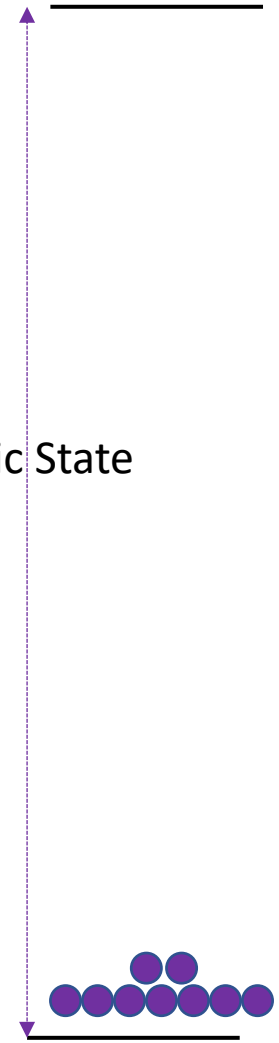


Nuclear spin

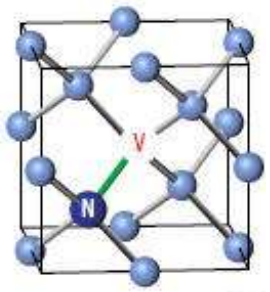


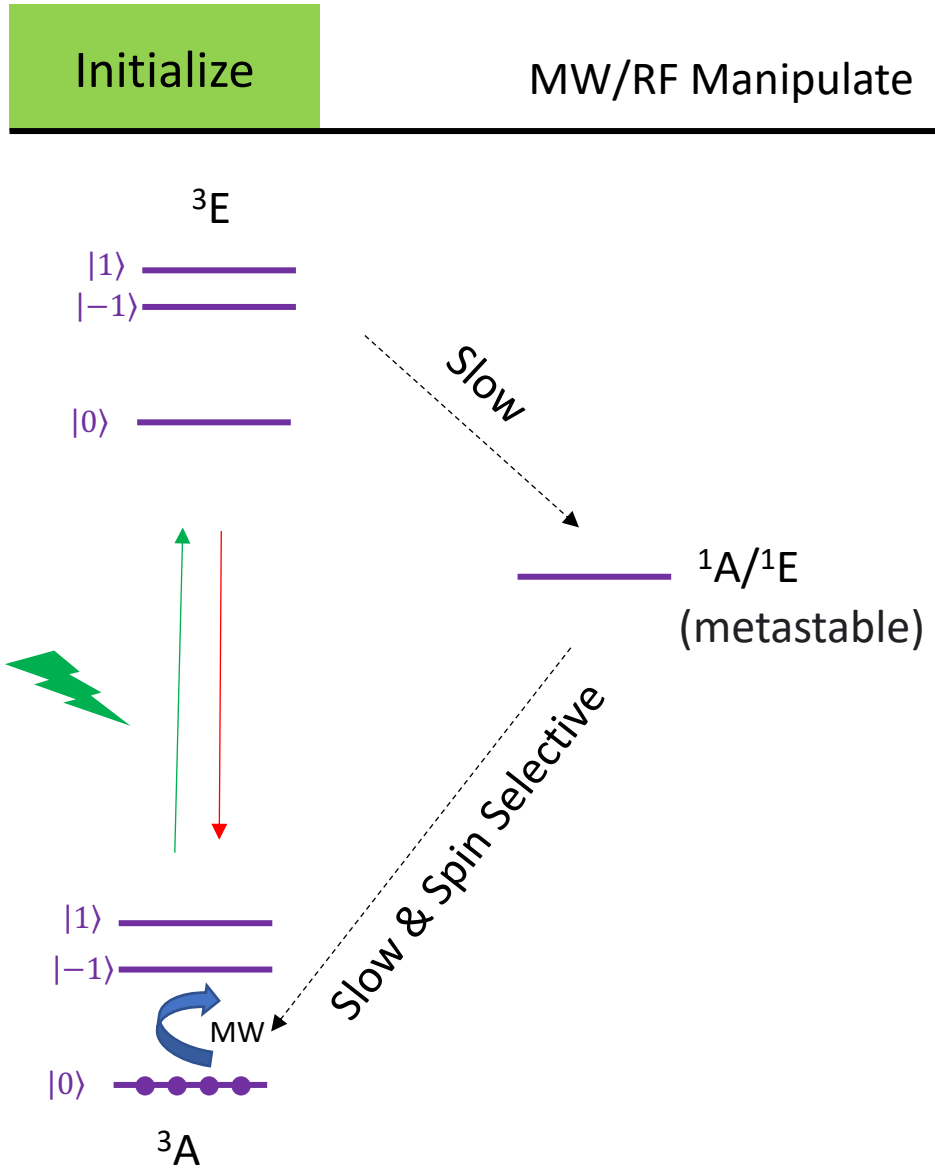
Electron spin

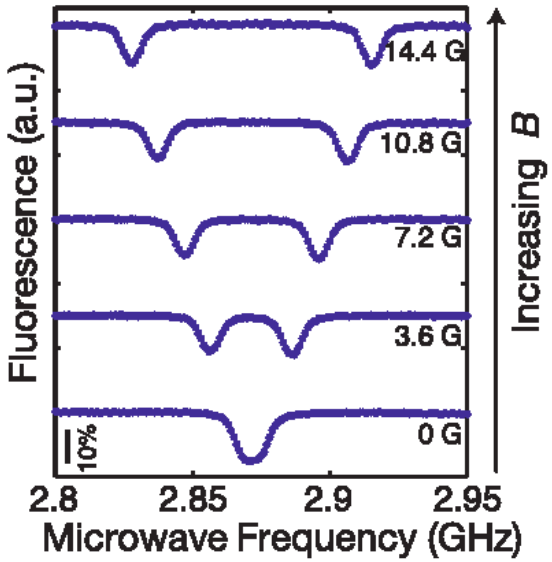
❖ **Best Initialization**



Spins (NV Diamonds)

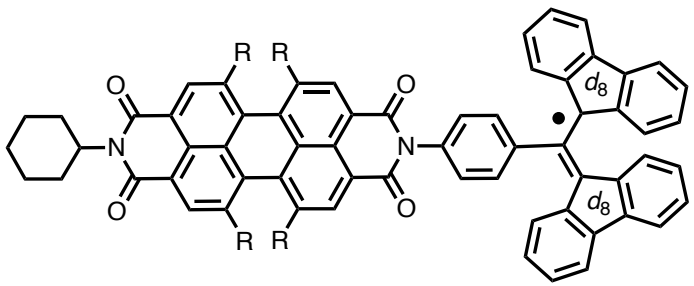


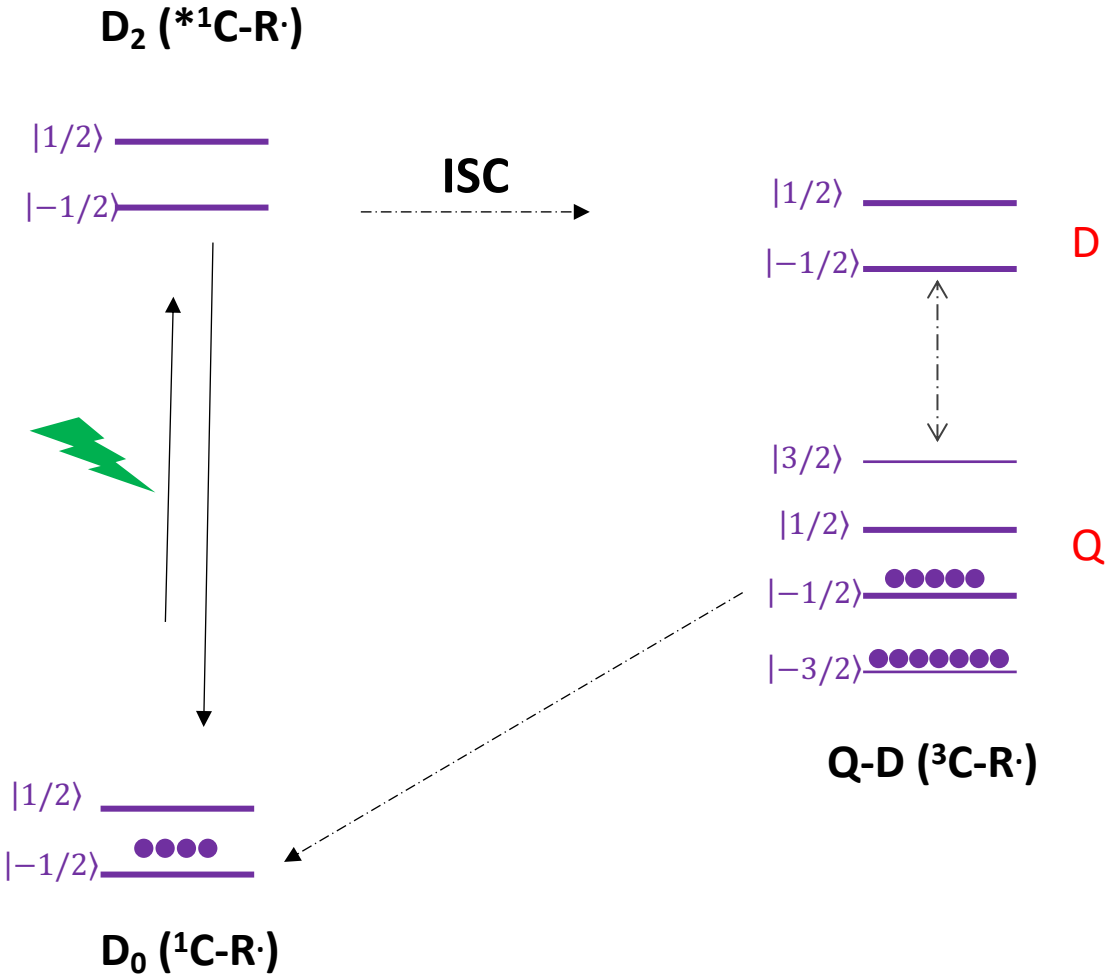




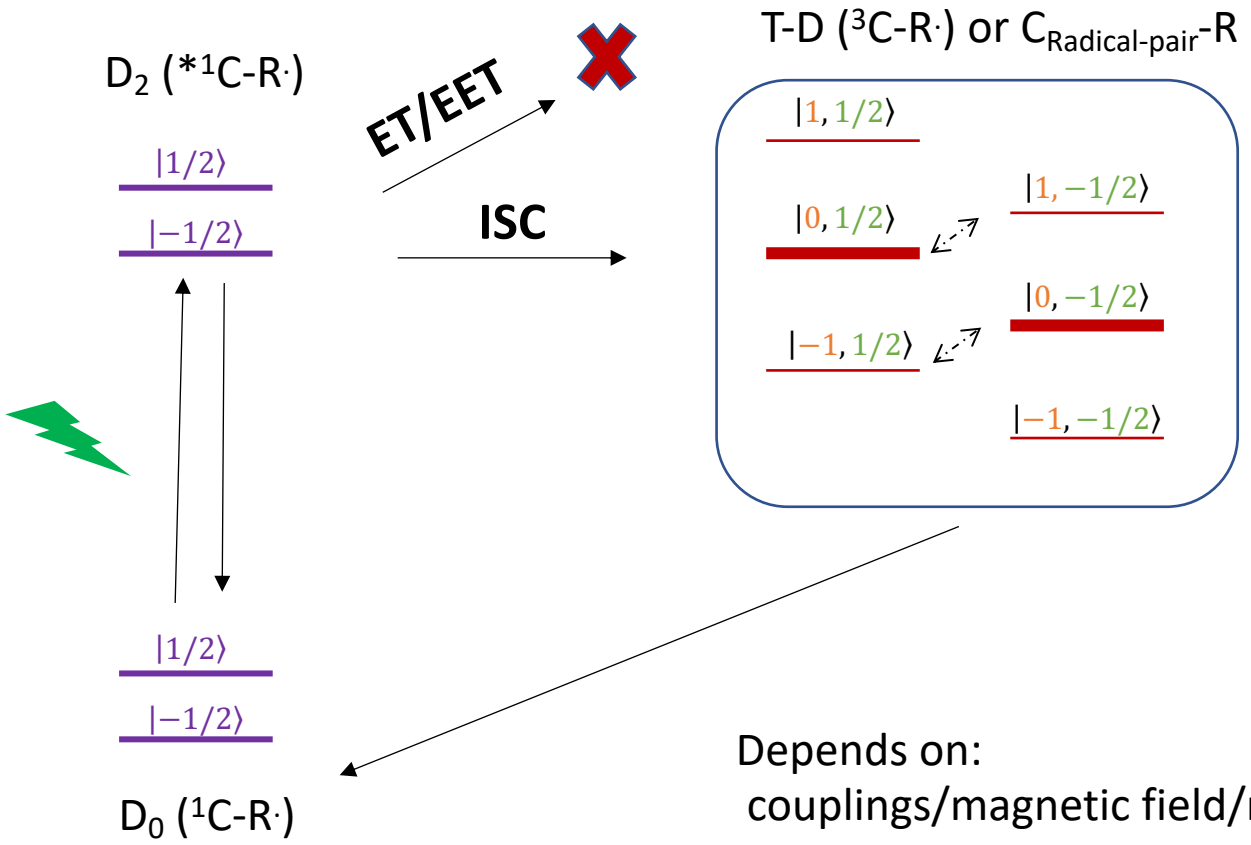
- High Sensitivity
- Long Coherence
- **Not scalable**

Molecular Analogue of NV centers





Light activated Chromophore + Radical

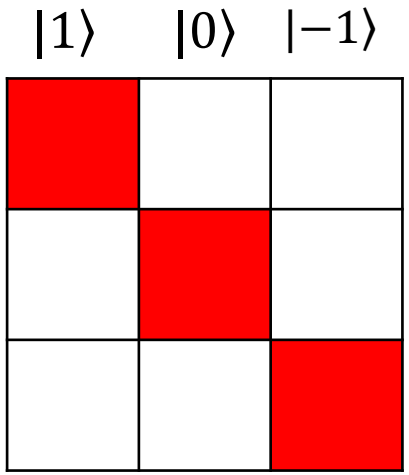


- Chromophores:
  Porphyrins; Perylene; PXX; PDI.
- Radicals:
  Nitroxides; Trityl; BDPA

Depends on:
couplings/magnetic field/molecular orbital symmetry

Light activated Chromophore + Radical

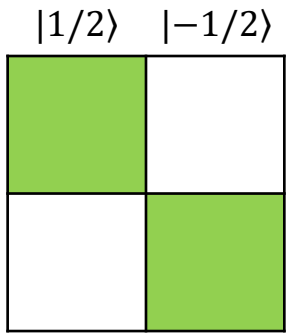
Matrix Representation



Spin -1

chromophore

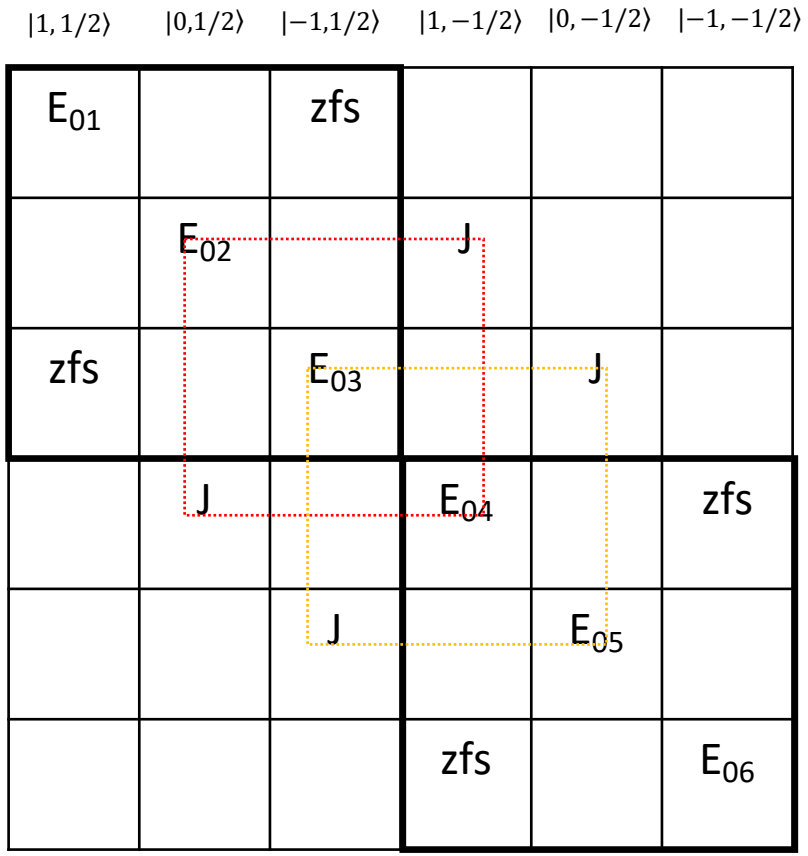
$\otimes$



Spin -1/2

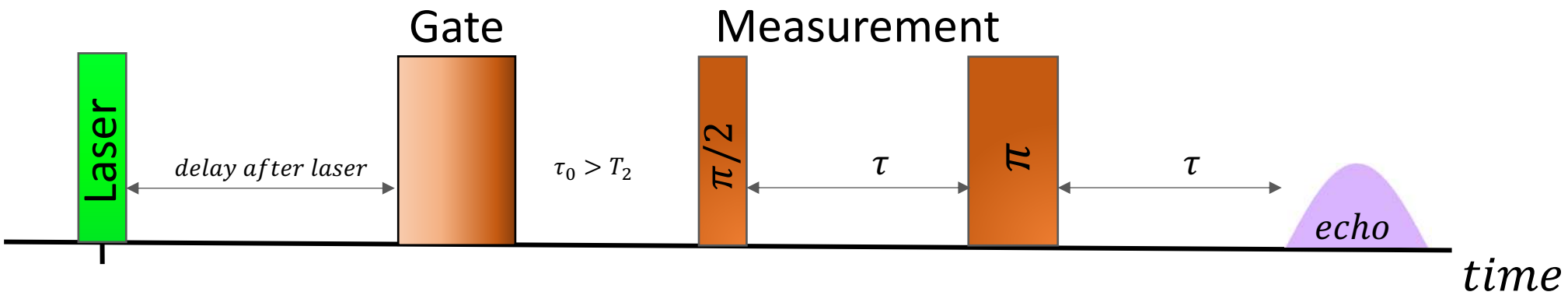
radical

Product basis →

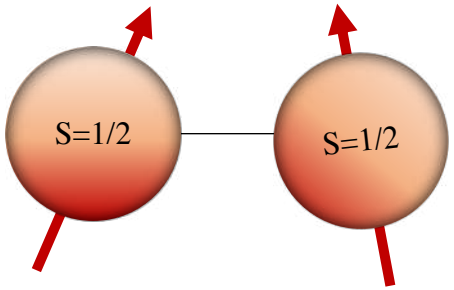


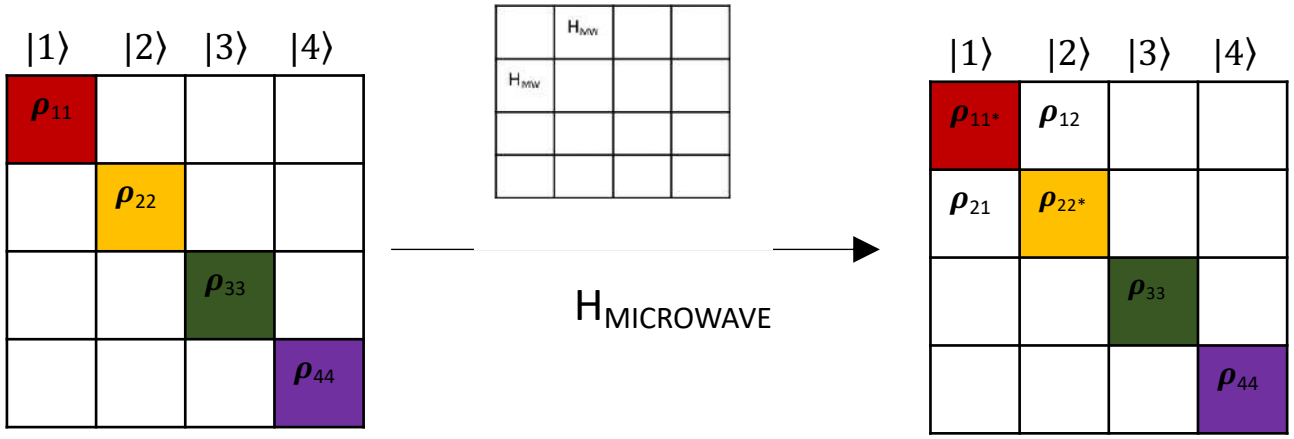
Spin 1 + Spin 1/2

Optically Pumped Molecular Spin Qubits

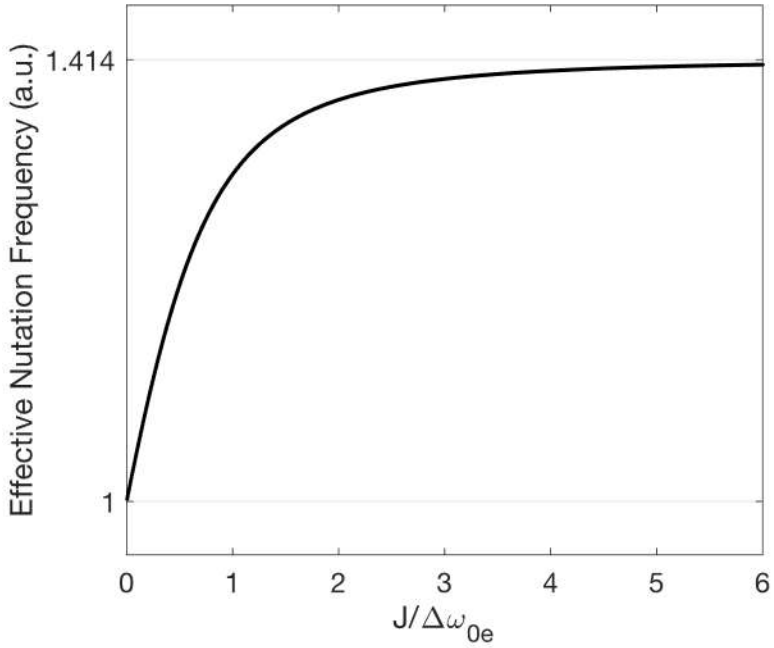


Effective Nutation

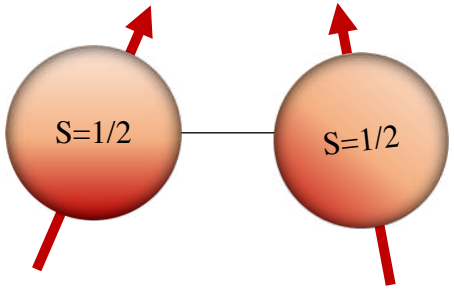




Radical Pair Triplet

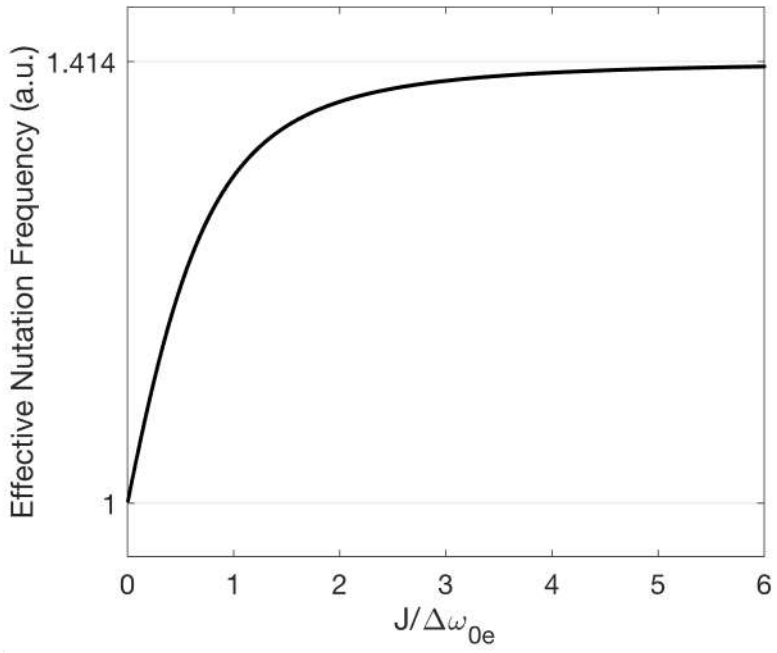


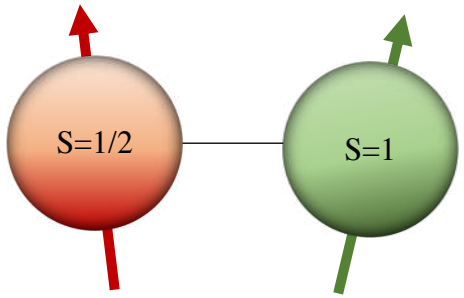
Effective Nutation



Radical Pair

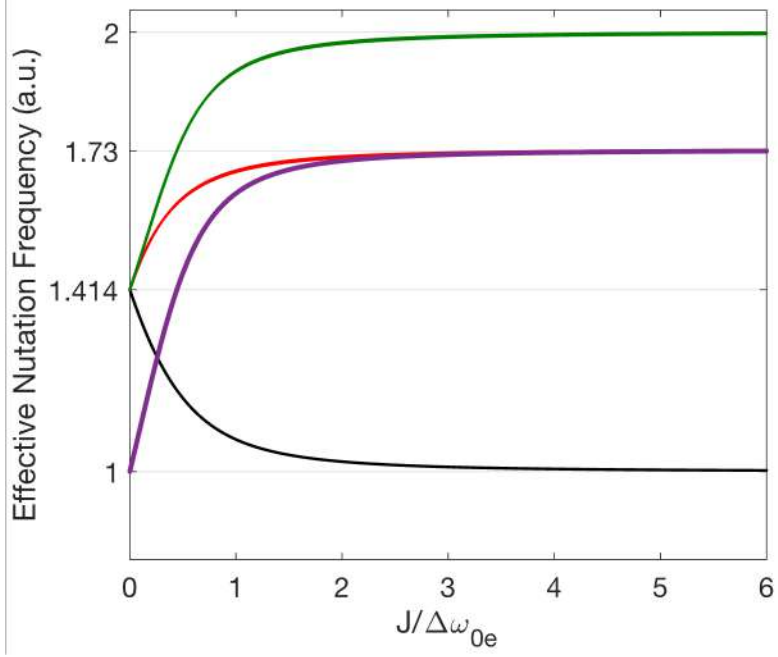
Triplet





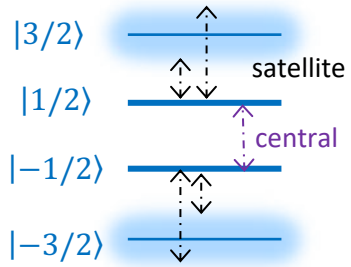
Triplet + Doublet

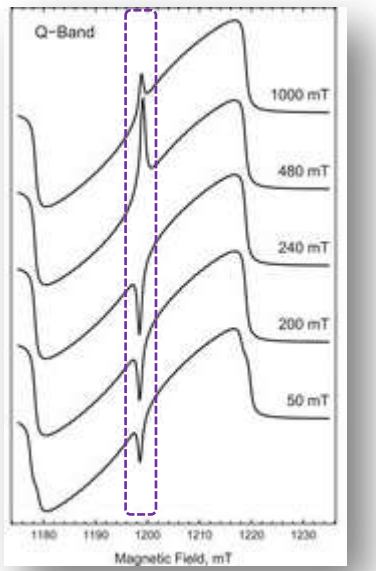
Quartet +Doublet



Molecular Spin Qubit Characterization

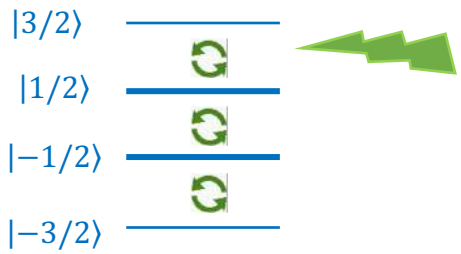
1. Narrow central transition: $|1/2\rangle \leftrightarrow |-1/2\rangle$



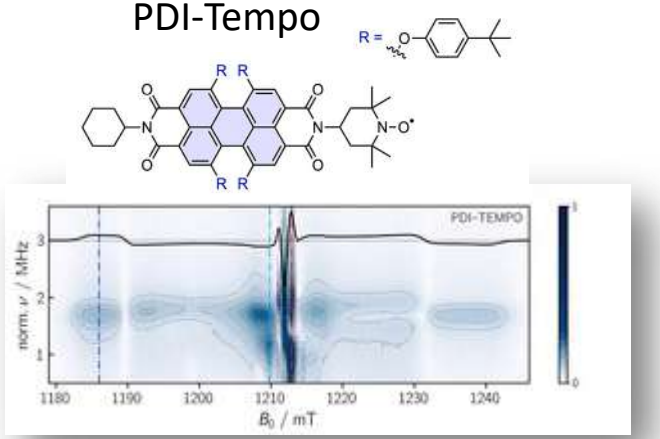


2. Nutation: $|m_s\rangle \leftrightarrow |m_s \pm 1/2\rangle$

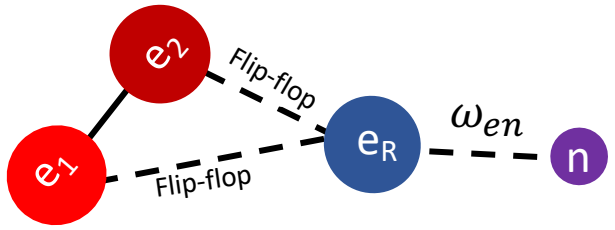
$$I^{\pm}|m_s\rangle = \sqrt{(I(I+1) - m(m \pm 1))}\,|m_s \pm 1/2\rangle$$

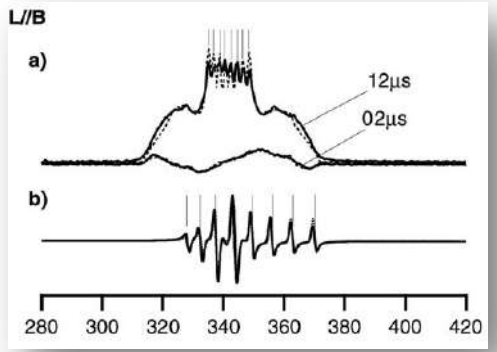


PDI-Tempo



3. Hyperfine splitting pattern



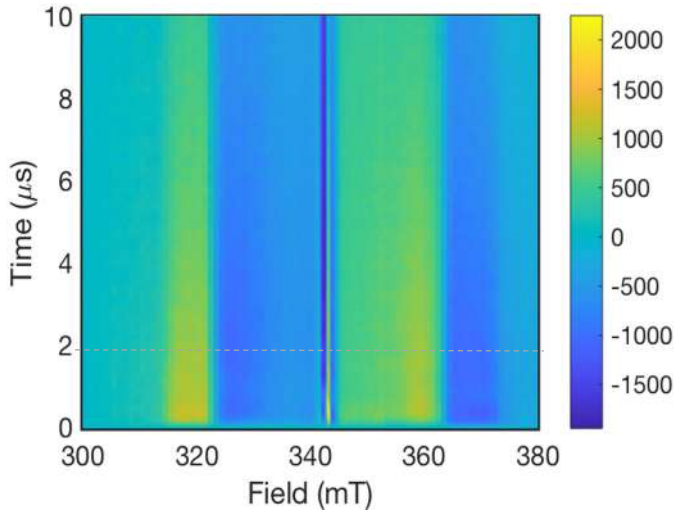


excited $e_1e_2e_s$-n

ground- e_s-n

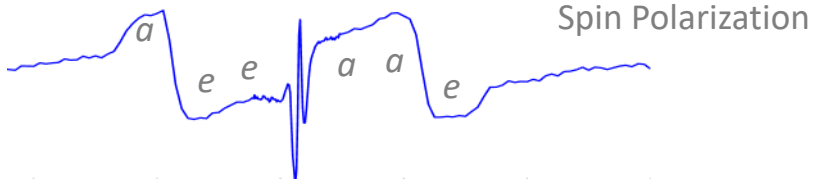
Case study

PDI-TEMPO @ 85 K



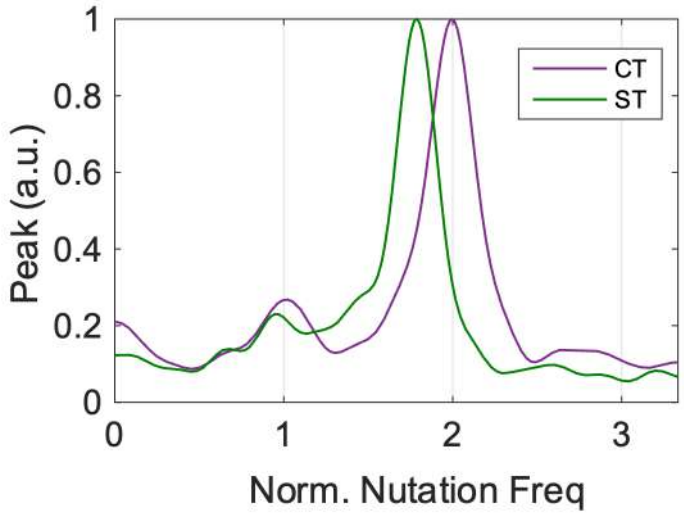
Hyperfine = $A_{14N}/3$

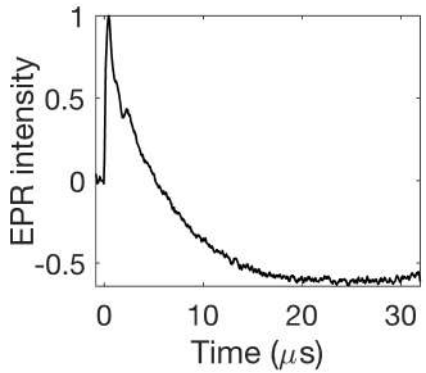
Satellite Central Satellite



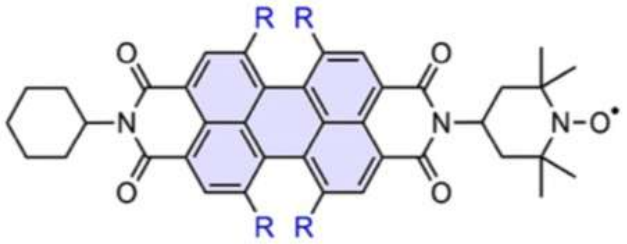
Spin Polarization

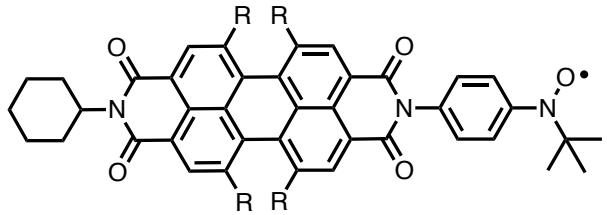
Nutation @ Central



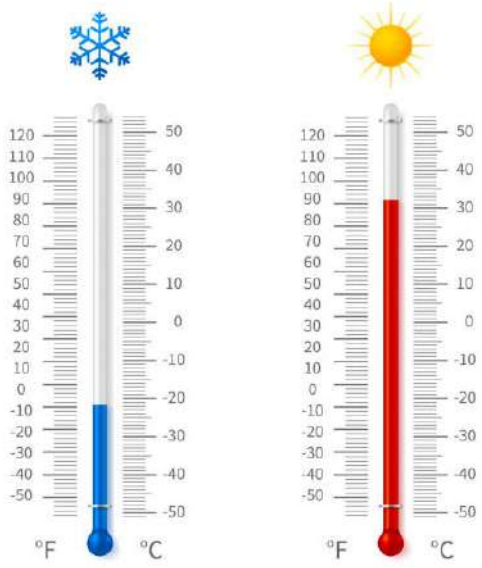


PDI- Nitroxide: TEMPO vs. BPNO





	PDI-TEMPO	PDI-BPNO
292 K	Small polarization	Large polarization (Quartet)
85 K	Large polarization (Quartet + Mixture)	Small polarization (Quartet)



- High temperature/ high field → Strong Coupling
- Low temperature/low field → Moderate Coupling

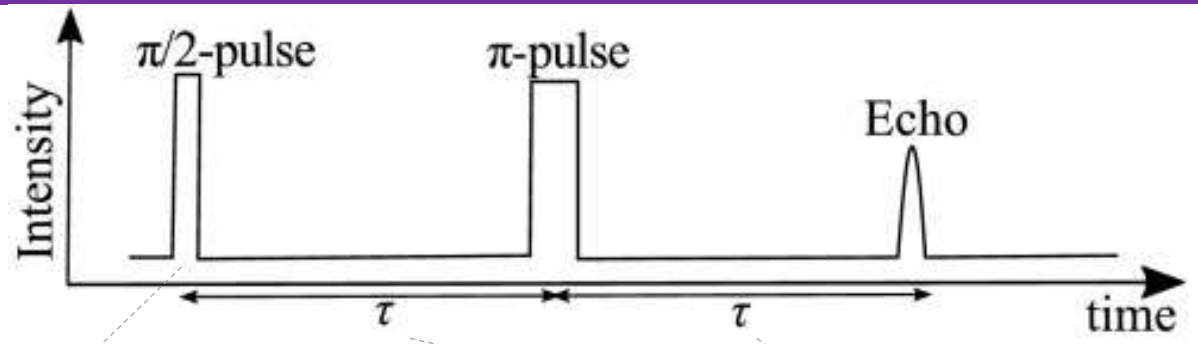
❑Spin Polarization

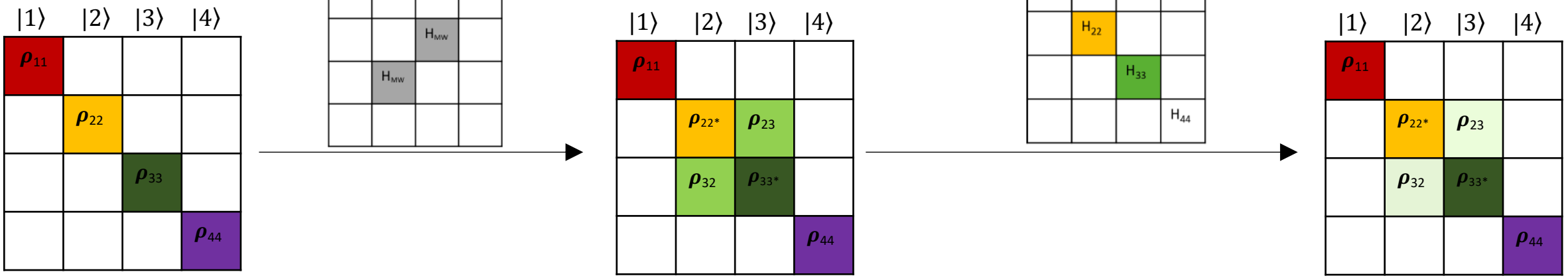
❑Spin Coherence

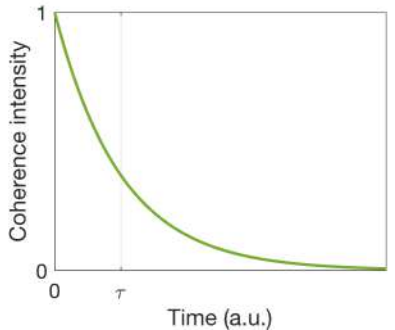
Solving one problem creates another!

1. Molecular Stability, Felxibity → Scalable
2. Low polarization → Initialization is an issue → Only Pseudo-initialization possible
3. Slow Relaxation → Long decoherence times
4. Coupled system → Universal
5. Heteronuclear → Specific measurement

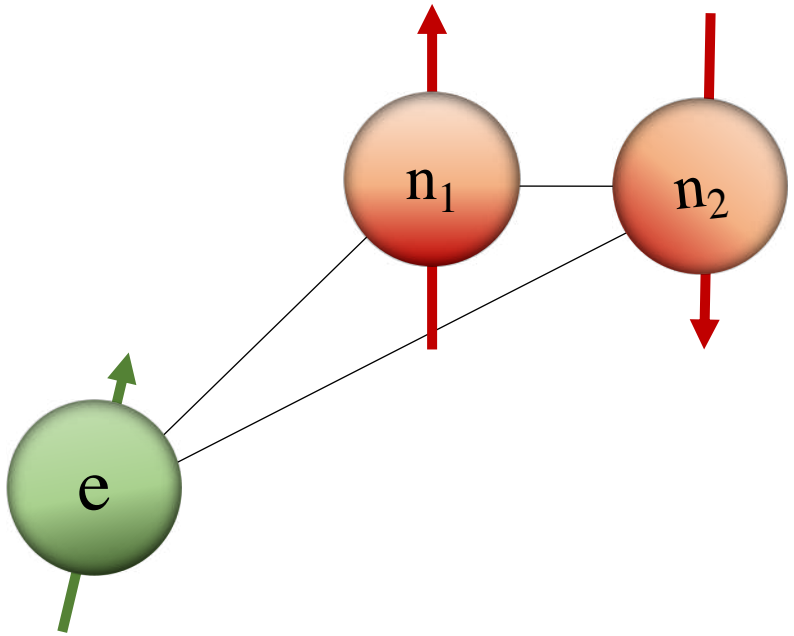
Coherence time: determines fidelity of a quantum gate





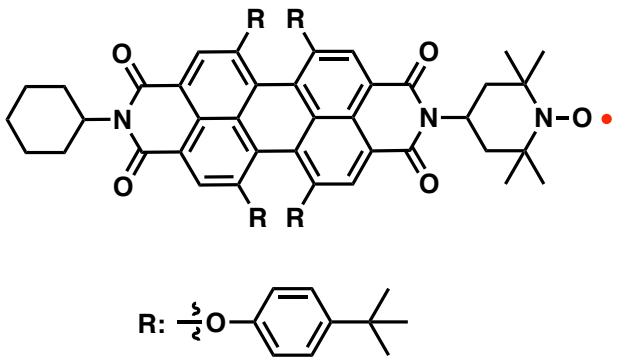


Decoherence mechanism

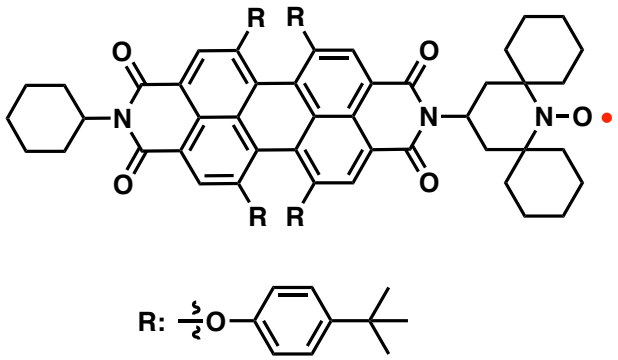


- Nuclear spin flip-flop or exchange is a dominant mechanism
- It changes the local magnetic field at e-spin site -> diphase the coherence
- Methyl rotation

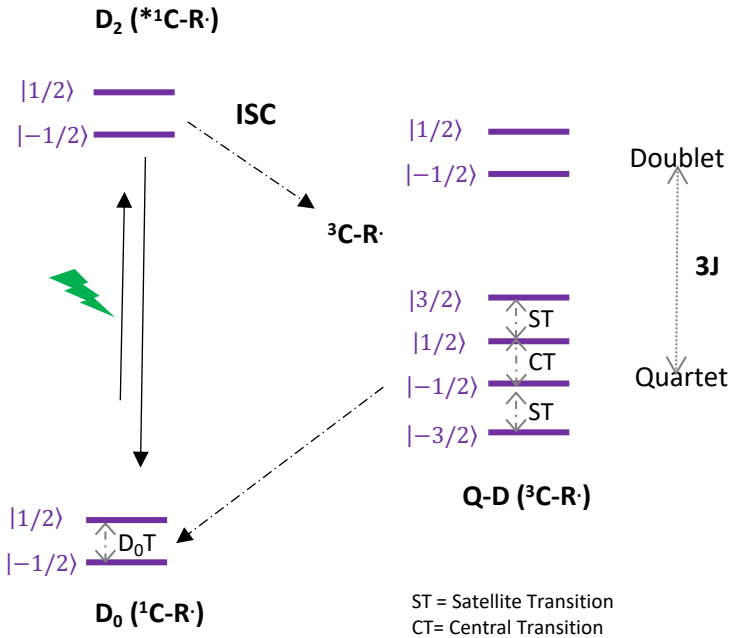
Systematic molecular design



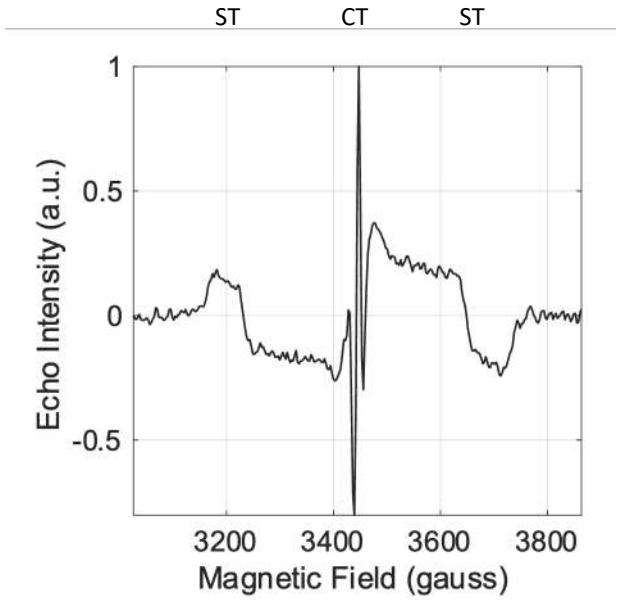
Molecule-1



Molecule-2



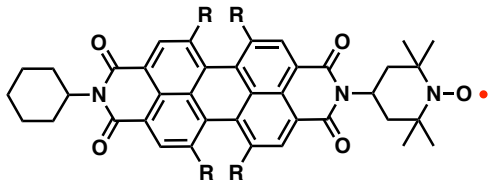
ST = Satellite Transition
CT= Central Transition
D_0T= Doublet Transition (Ground state)

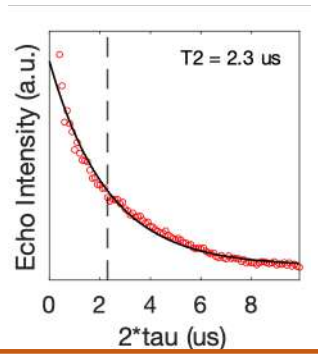


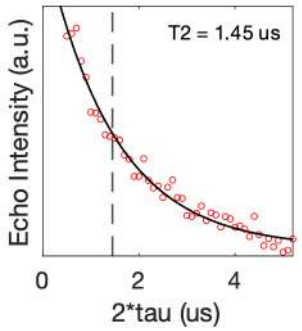
Longer decoherence time for Molecule-1

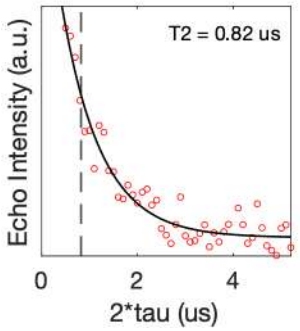
Doublet Transition (D_0) **Central Transition** **Satellite Transition**

Molecule-1

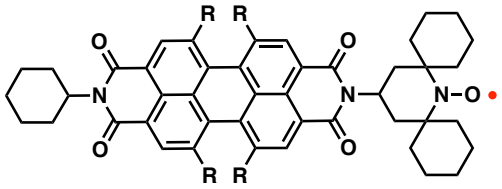


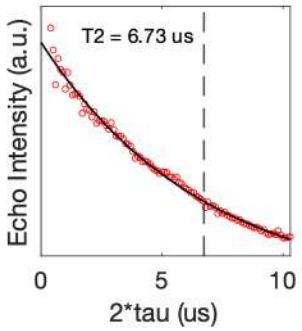


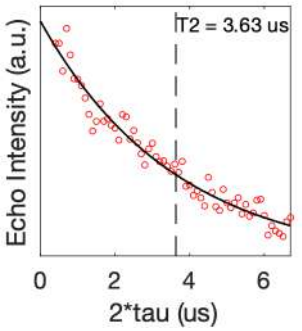


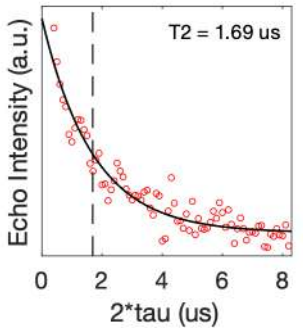


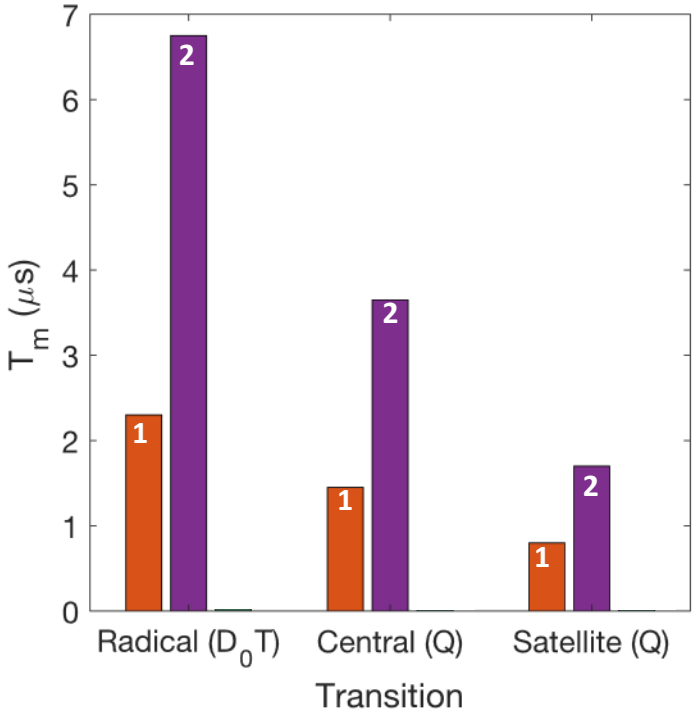
Molecule-2











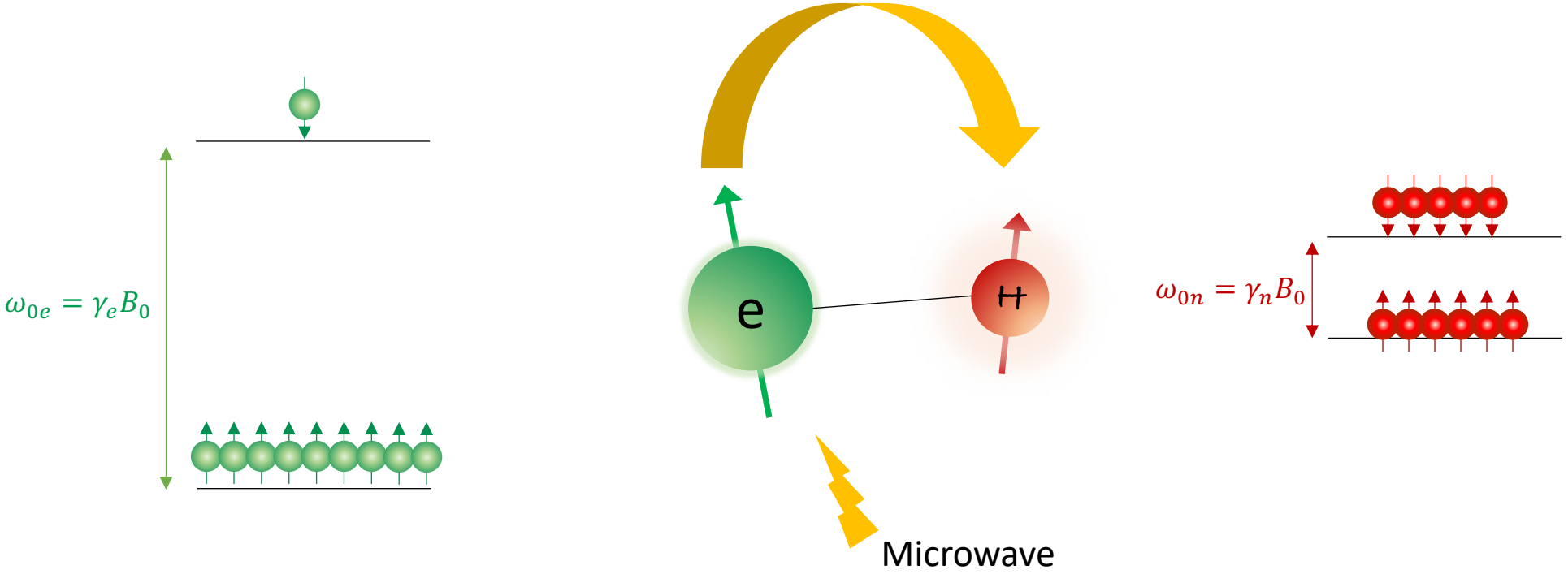
We **improved** the (SQ) coherence time by a **factor of 2** while retaining key quartet features.

❑Spin Polarization

❑Spin Coherence

❑Polarization storage

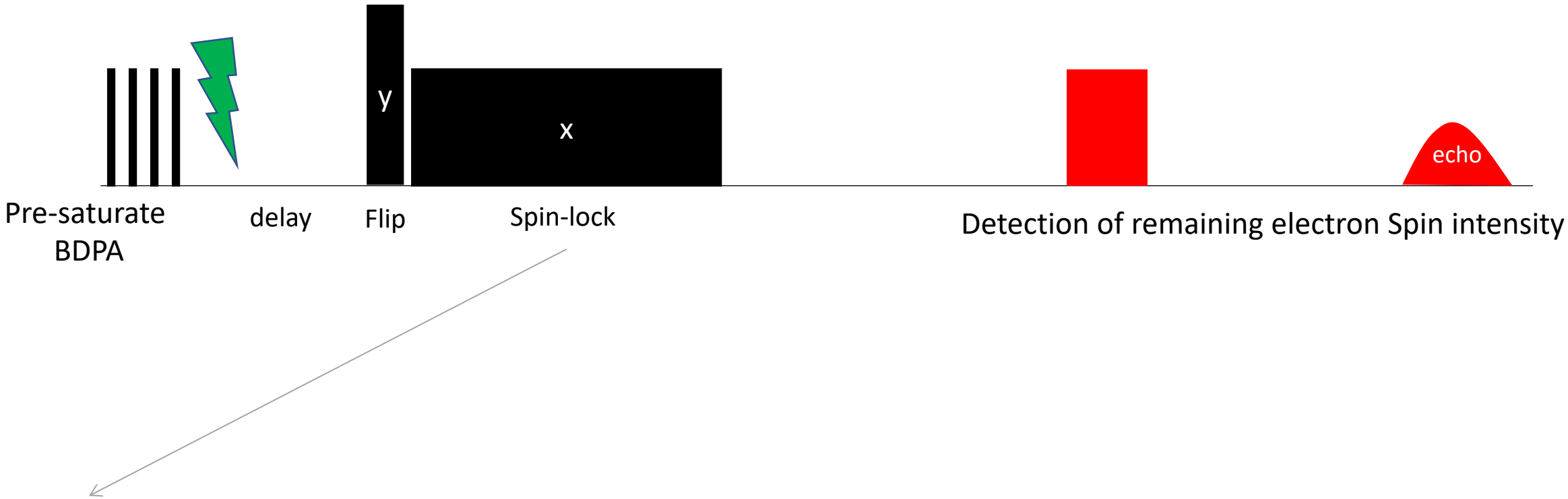
Polarization Transfer & Storage



$$\omega_{oe} \gg \omega_{on}$$

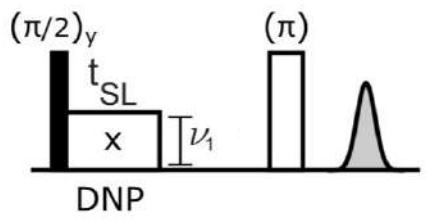
- Direct e-n flip-flop is not possible (energy non-conserving process)
- Dressed electron spin state using microwave irradiation.
- Several applications in NMR and MRI.

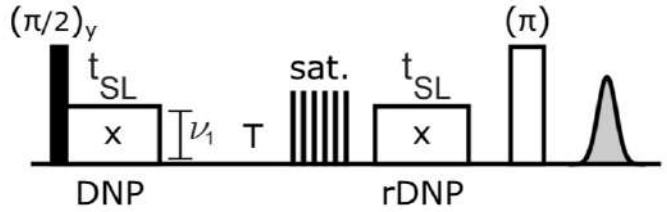
Polarization Transfer Using Organic Chromophore

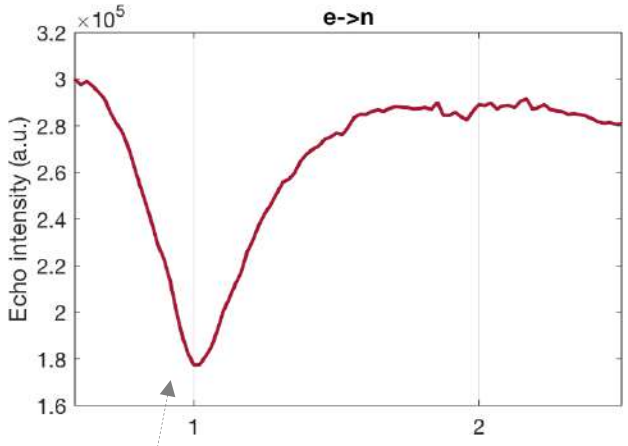


***Key concept**: Match effective field on "dressed" electron spin with nuclear larmor frequency*

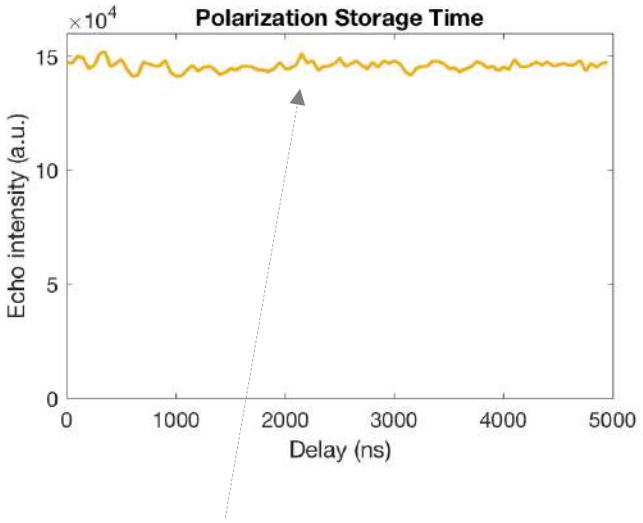
Quantum Memory: {e→n → store→ n→e}
Or Hyperpolarization using pre-hyperpolarized electron spins

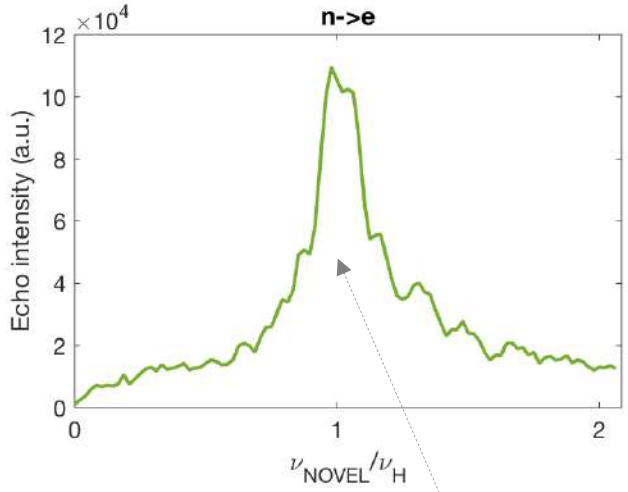






MW Nutation/Nuclear larmor



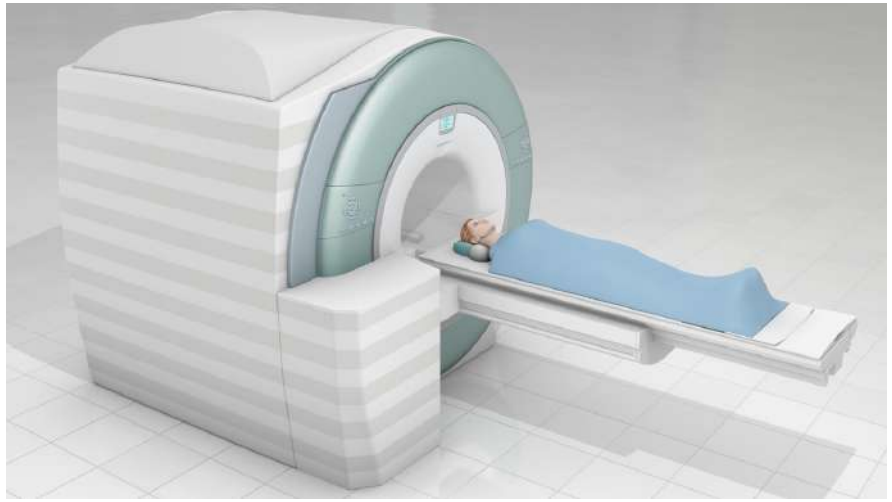


Polarization transferred to nucleus

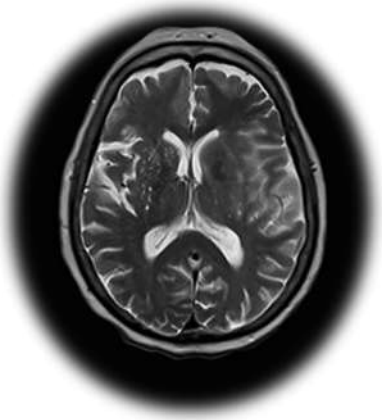
Polarization stored on nucleus

Polarization relayed back to electron

Other applications of optically pumped molecular spin qubits



❖ MRI -Sensing



Why?

- More sensitive detection.
- Saves time by orders of magnitude.

Take Home

- ❑ Spin Polarization: optical pumping
- ❑ Spin Coherence: minimize nuclear spins flip-flop
- ❑ Polarization storage: e ←→ n (transfer, store, reverse transfer)