



INSTITUTE FOR TERAHERTZ
SCIENCE AND TECHNOLOGY

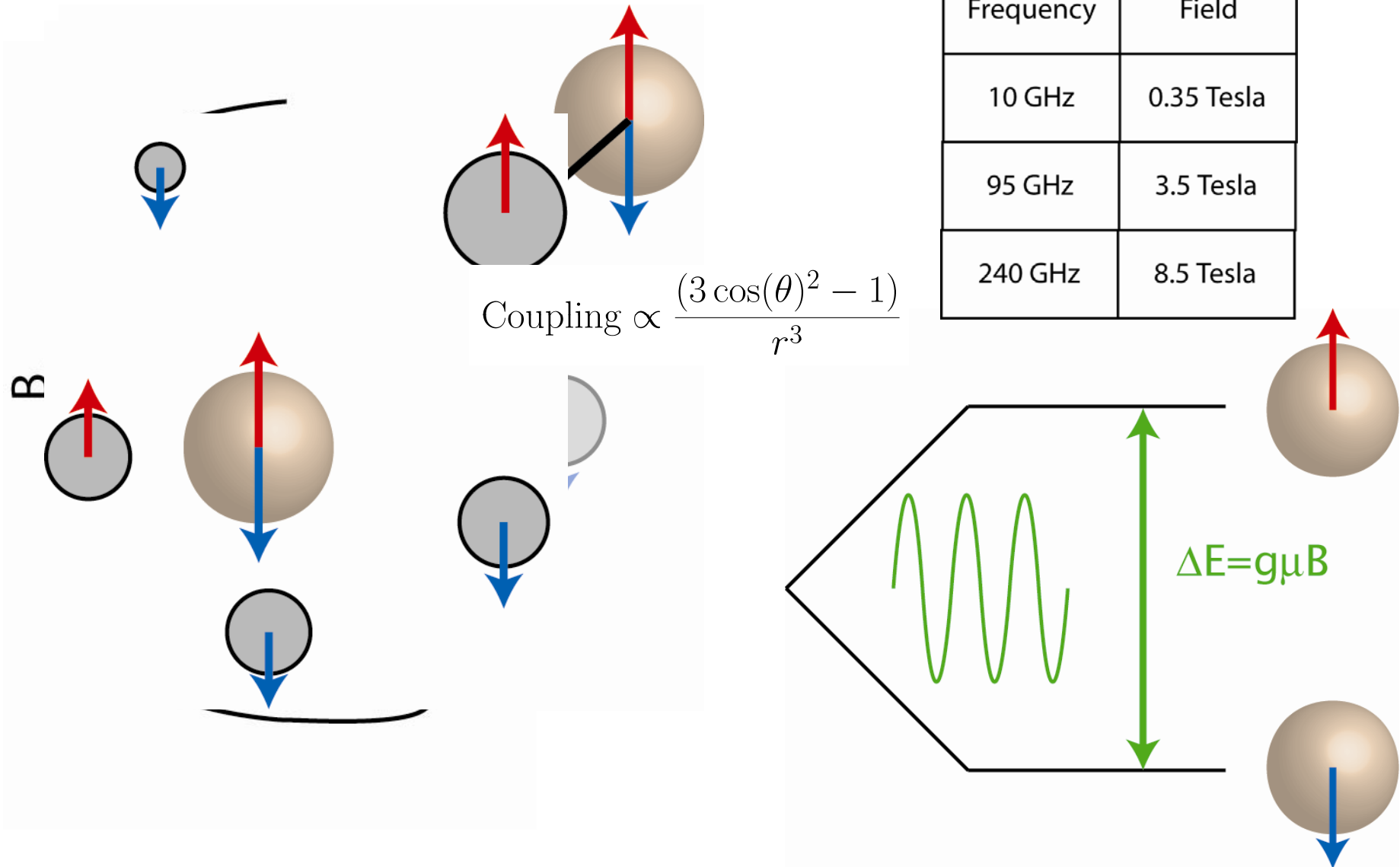
Gd³⁺-Based Spin Probes for High Frequency Electron Paramagnetic Resonance

Devin Edwards, Daniella Goldfarb, Song-I Han, Mark Sherwin

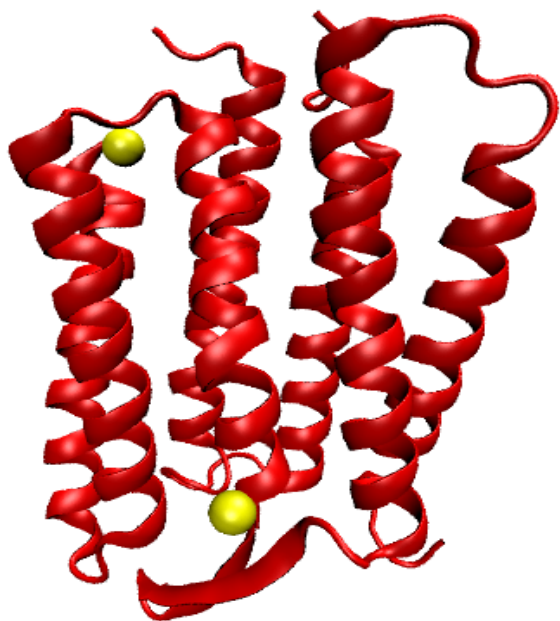
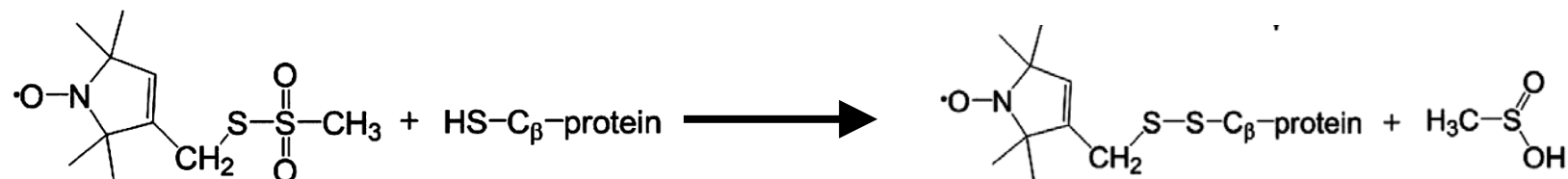
ITST Seminar

October 6th 2011

Paramagnetic Species Probe the Local Environment



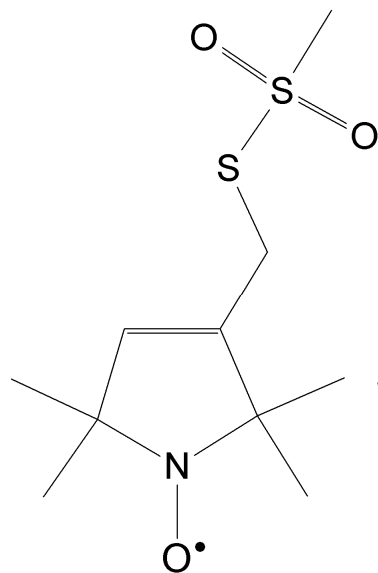
Biological Distance Measurements with EPR



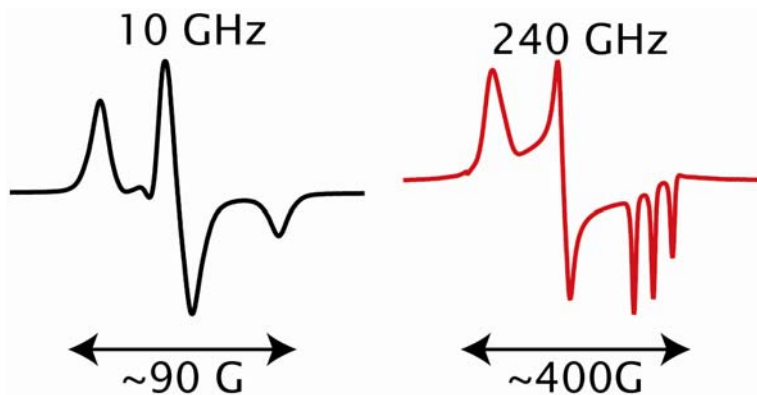
ProteoRhodopsin

Observing Long Distances with Gd^{3+} at High Fields

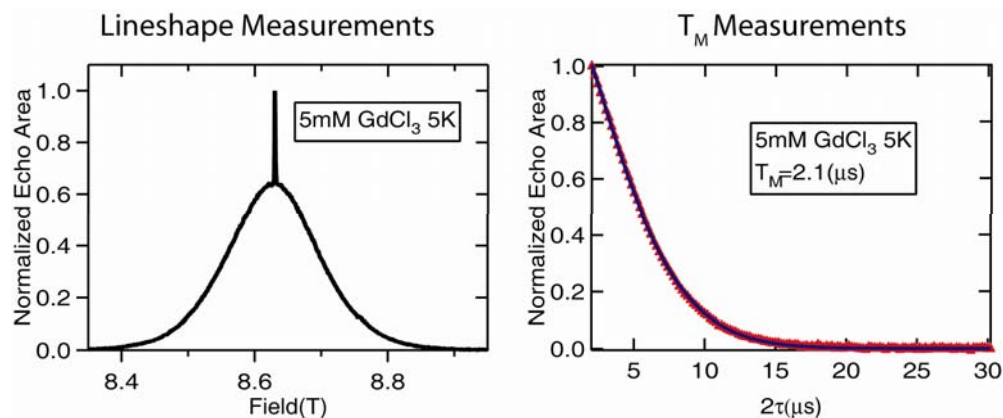
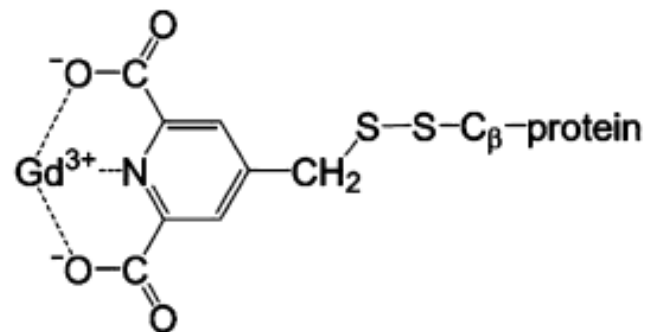
Nitroxide



Structure
Environment
Water Dynamics
Motion



Gd^{3+}

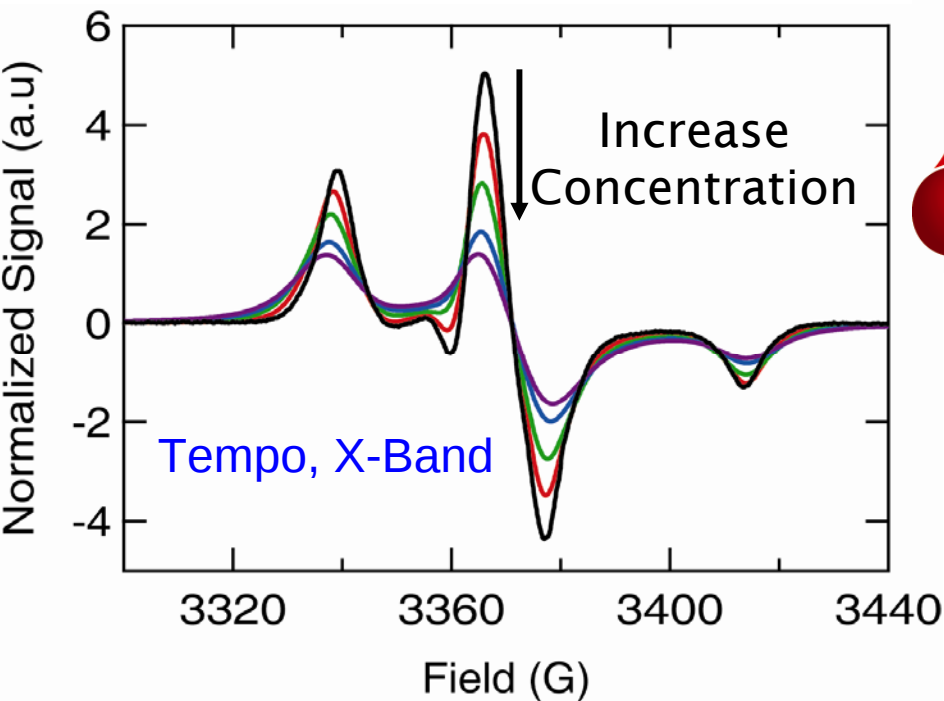


Su, X.; Otting, G.; et al. *JACS* **2008**, 130, (32), 10486-10487.

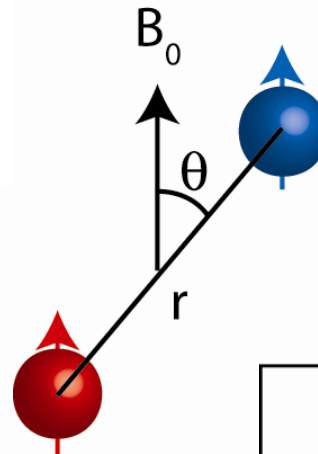
Potapov, A.; Goldfarb, D.; et al. *JACS* **2010**, 132, (26), 9040-9048.

Distance Measurement in EPR

Lineshape Analysis



**Quantifiable Distances
Nitroxides: 10-25 Å**



Double Electron-Electron Resonance

	CW Lineshape	Pulsed DEER
Ranges	1-2.5nm	1.5-8nm
Distribution Information	Some	Complete Profile
Broad Distributions	Yes	Difficult
Temperature	Frozen	Below 100K
Instrument	Low Power 1 Frequency	High Power 2 Frequency
Exp. Time	~Hrs	~Day

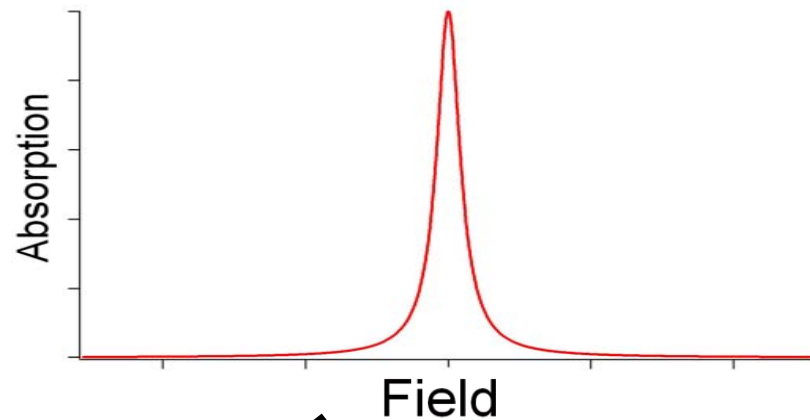
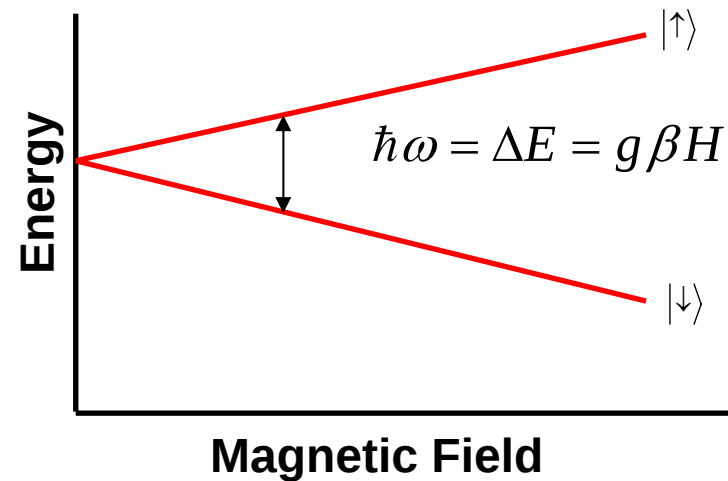
Steinhoff, H. J. et al., *Biophysical Journal* **1997**, 73, (6), 3287-3298.

Pannier, M.; Veit, S.; Godt, A.; Jeschke, G.; Spiess, H. W. *JMR* **2000**, 142, 331-340.

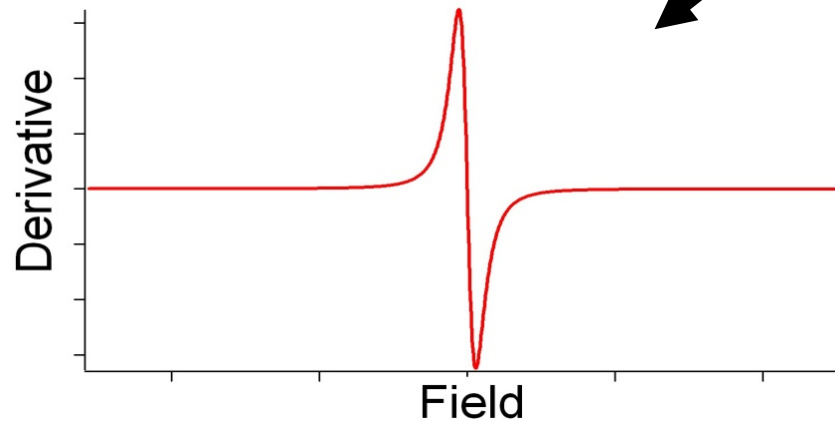
Continuous Wave(cw)-EPR

Fixed Frequency

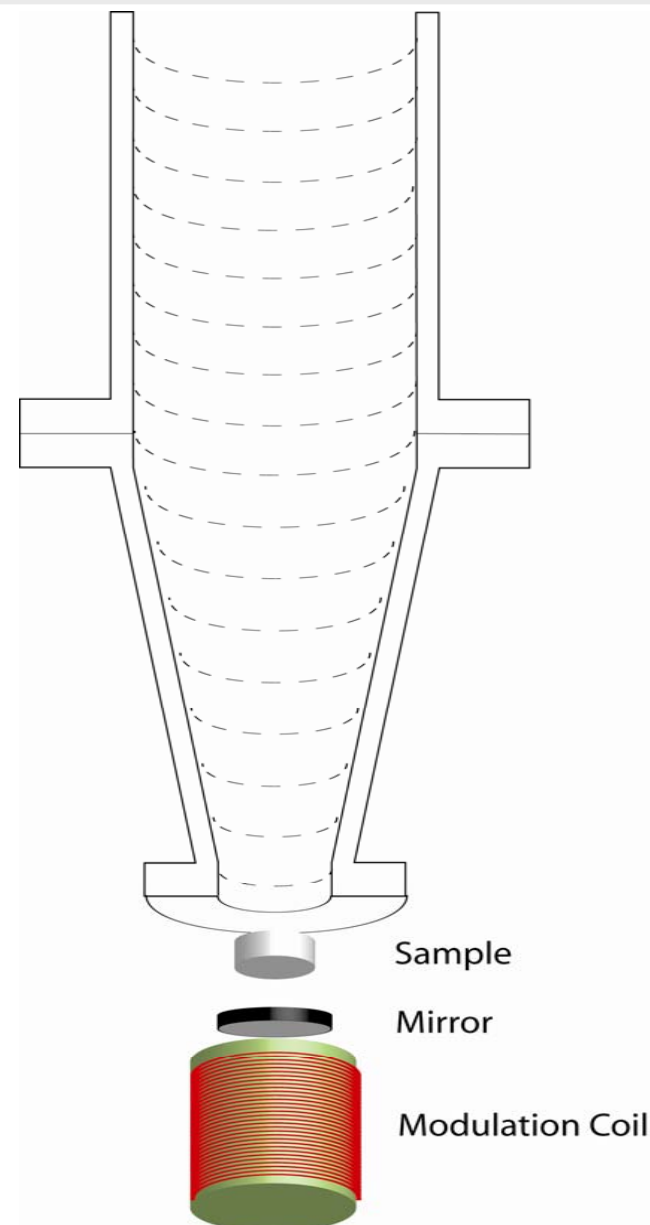
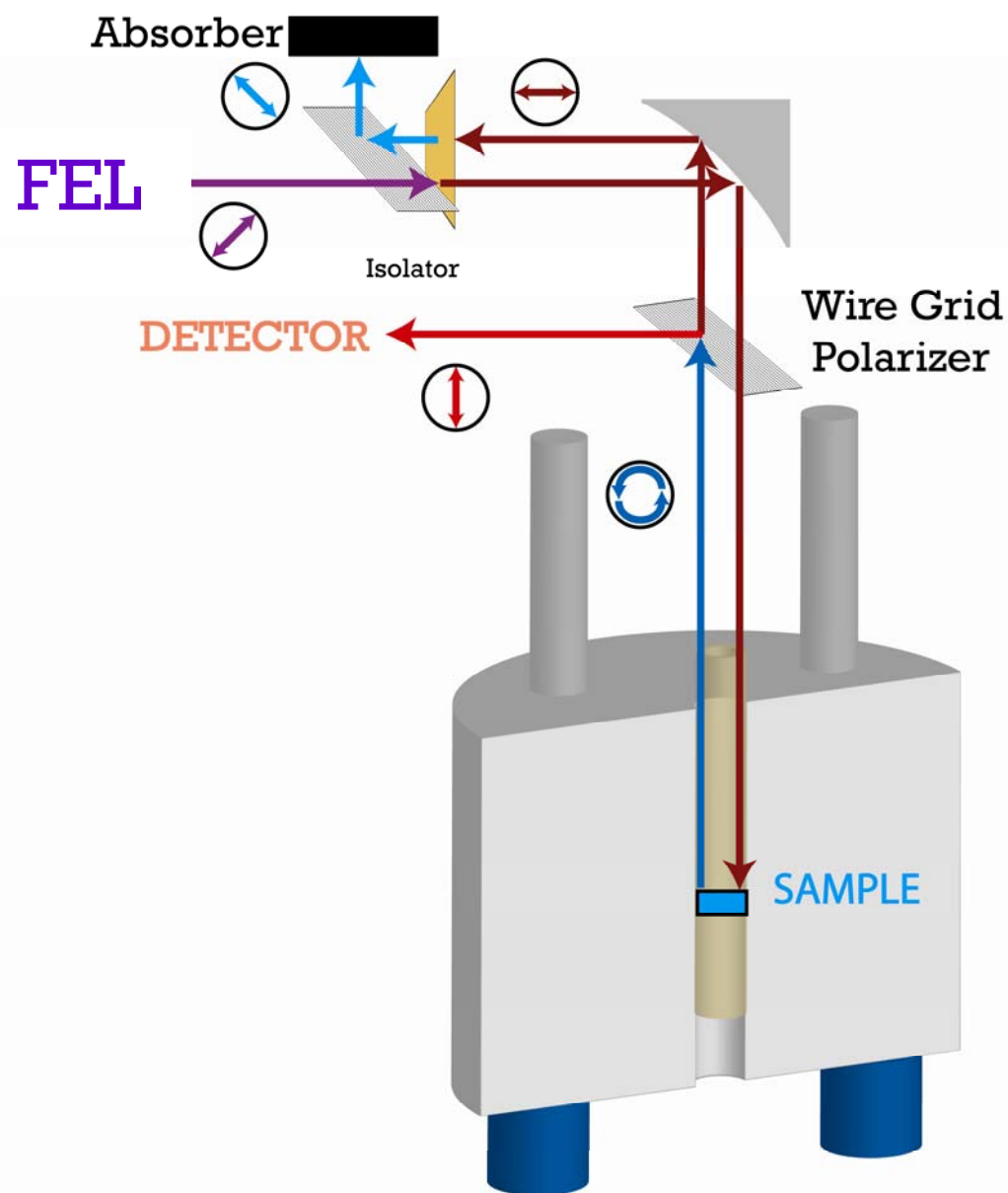
Sweep Field



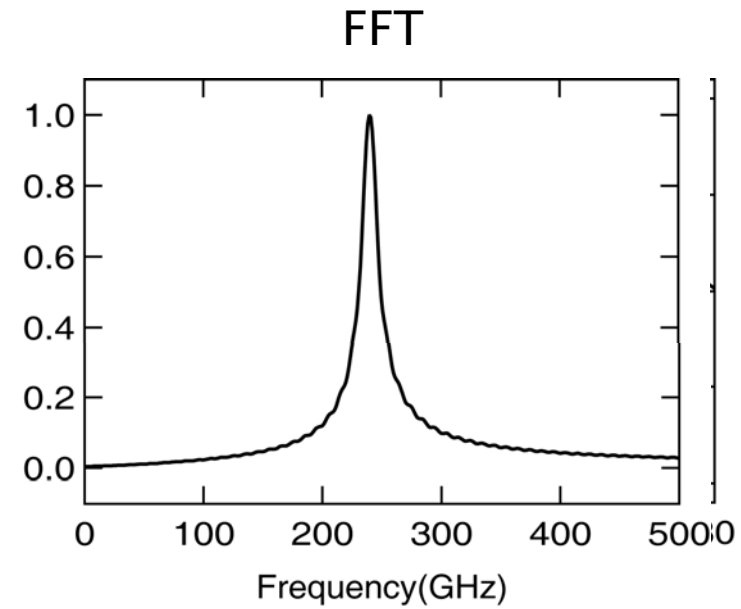
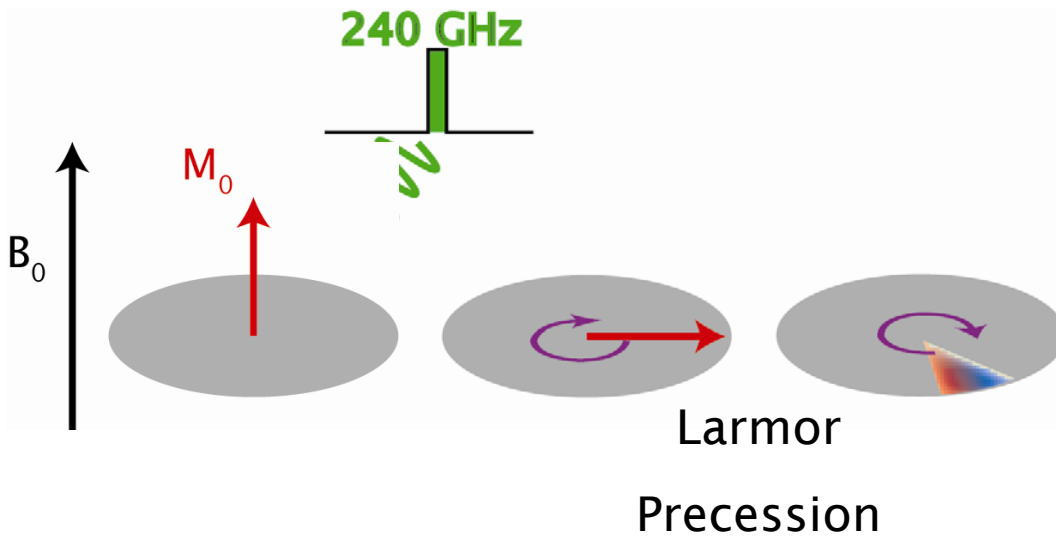
Field is
Usually
Modulated
During
Measurement



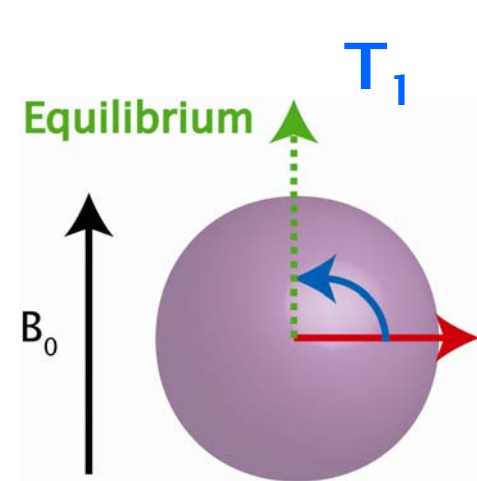
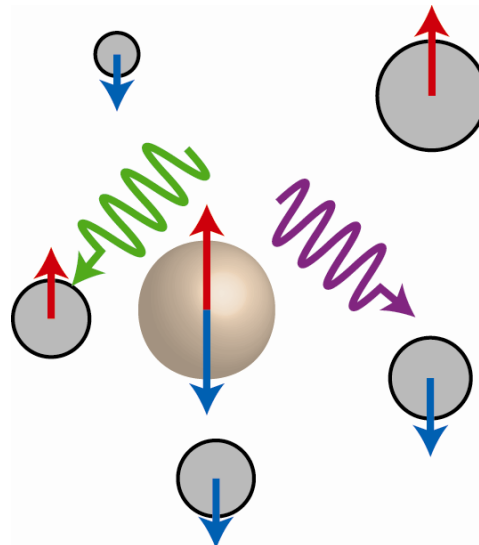
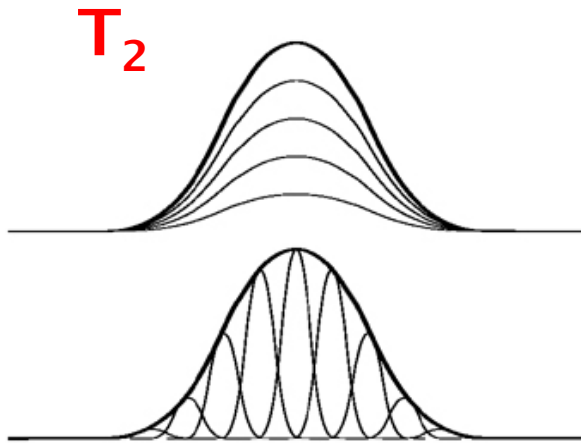
An EPR Spectrometer



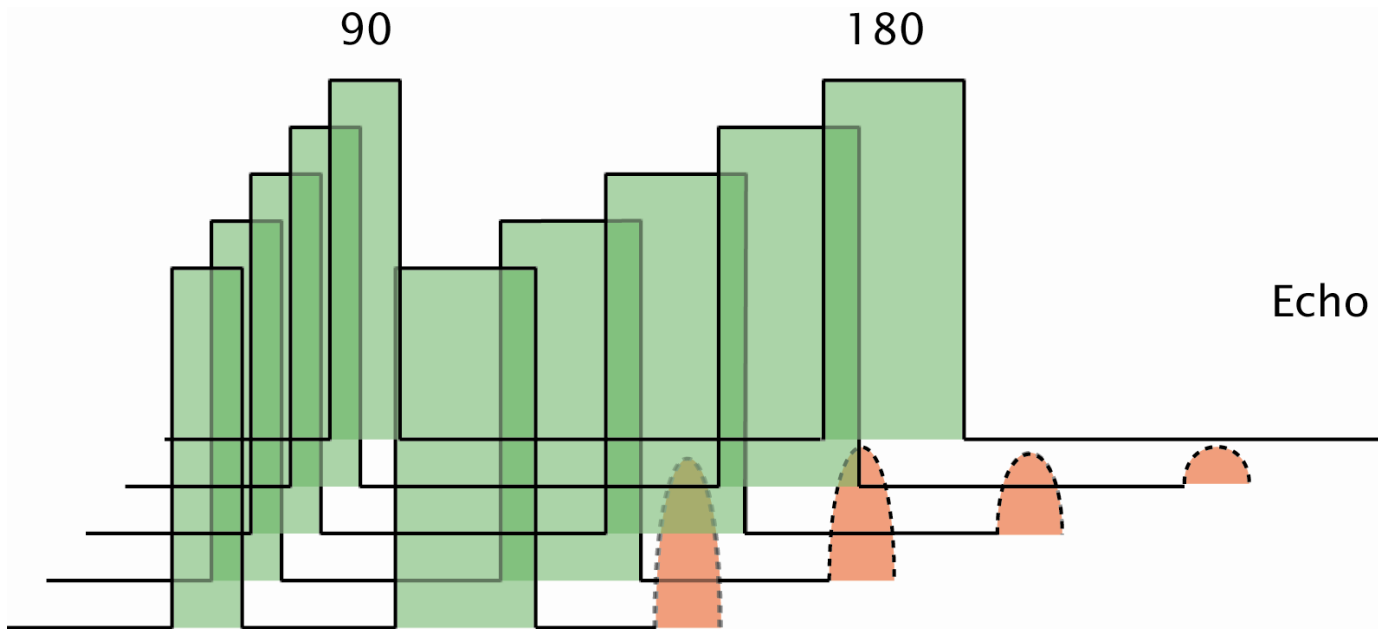
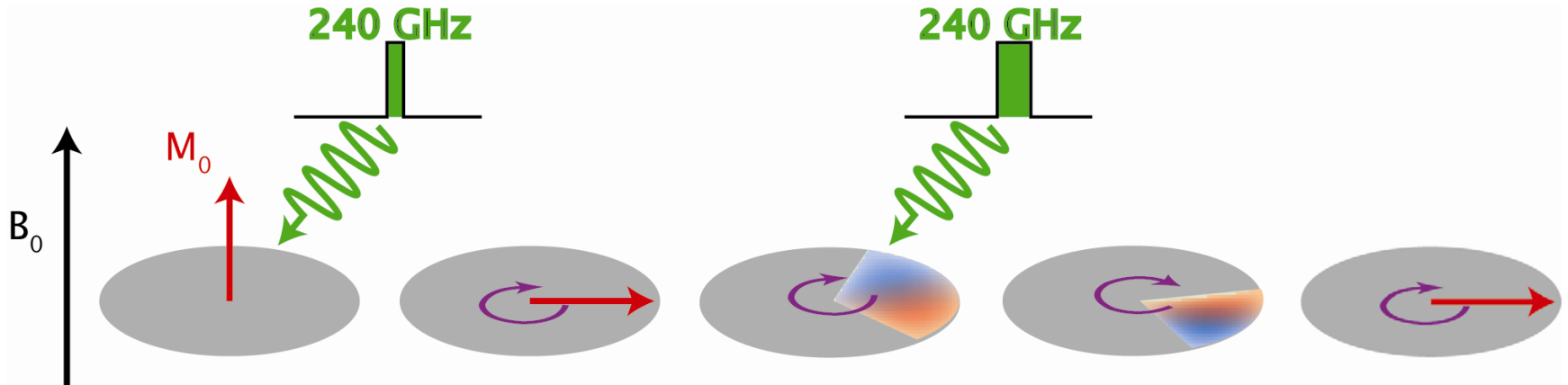
Pulsed EPR



Time Resolved/Multi-Frequency

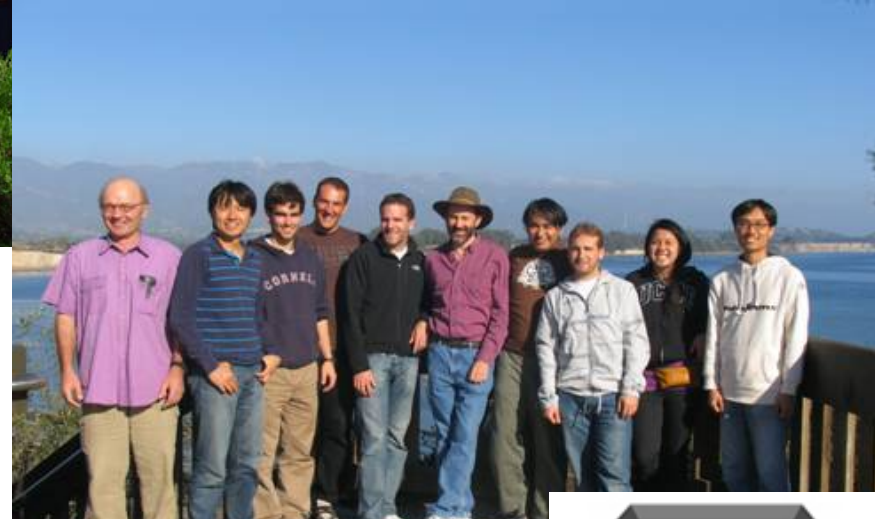


The Hahn Echo



Determine
Phase
Memory
Time (T_M)

Thanks!!



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Hamiltonian and the Spectra

$$\mathcal{H} = \underbrace{g\beta B_0 S_Z}_{\text{Zeeman}} + \underbrace{\vec{S} \cdot \bar{A}(\theta) \cdot \vec{I}}_{\text{Hyper fine}} + \underbrace{\vec{S} \cdot \bar{D}(\theta) \cdot \vec{S}}_{\text{Dipolar}}$$

