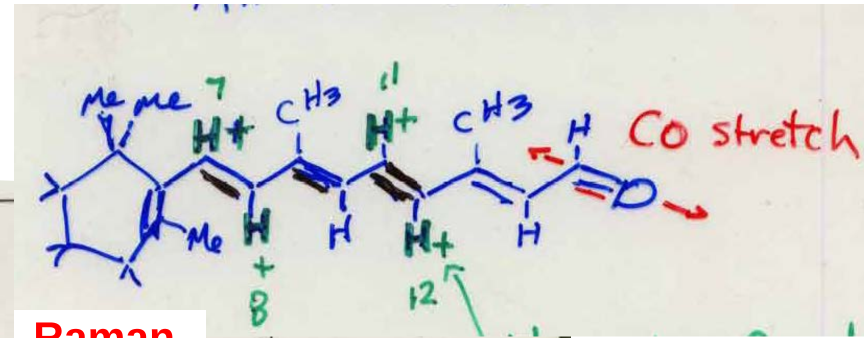


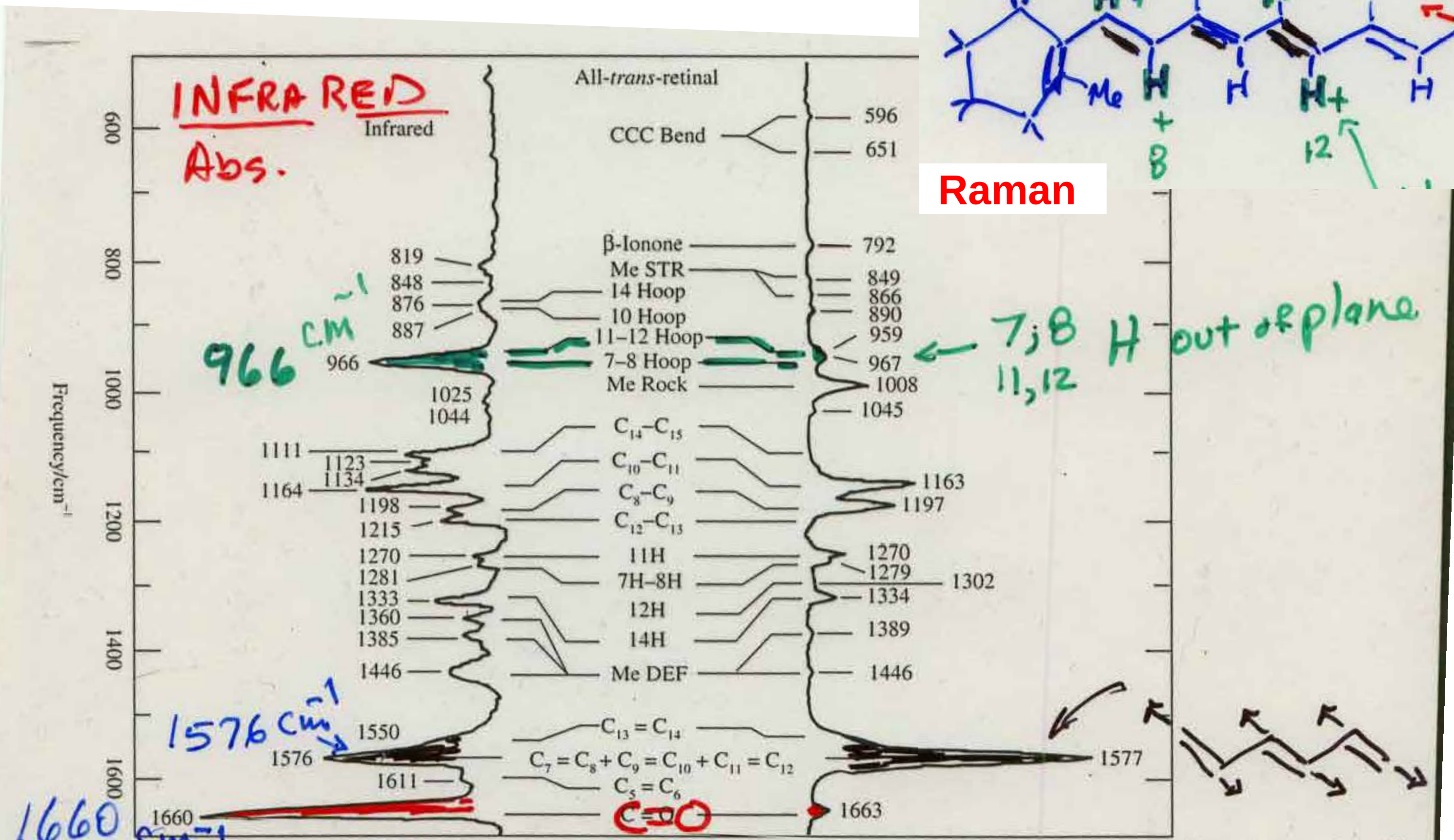


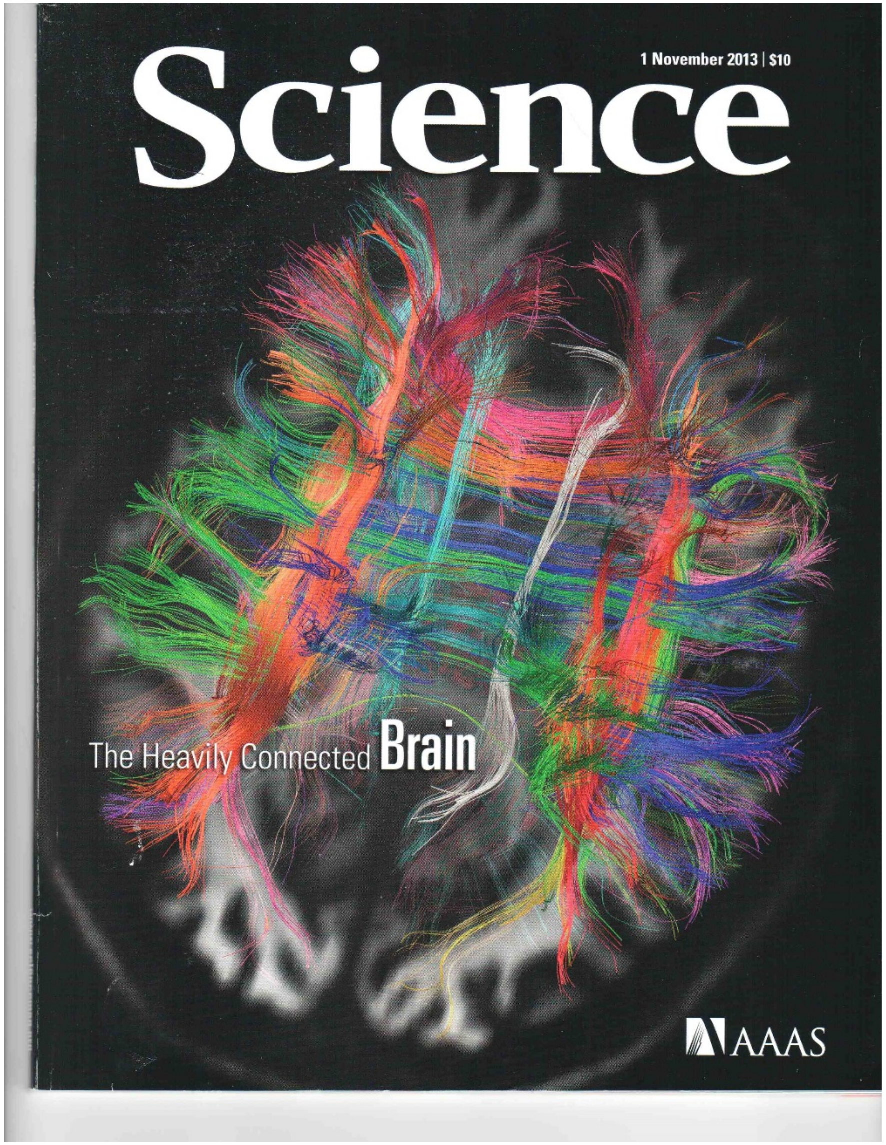
Fig. 13.36

Fig. ~~10.42~~ Raman and infrared spectra of all-*trans*-retinal in the region from 600 cm⁻¹ to 1600 cm⁻¹. The infrared absorbance is inverted to facilitate comparison with the Raman. The Raman spectrum was measured in CCl_4 using 676.4-nm excitation from a krypton ion laser. Solvent peaks were subtracted. The infrared spectrum was measured with a thin film deposited by evaporation from a pentane solution on a KBr window. All peaks have been assigned to particular vibrations of the molecule. Me STR, Me Rock, and Me DEF refer to the stretching, rocking and the deformation of methyl groups; Hoop means out-of-plane motion of H atoms. Note that double bond vibrations occur at higher frequencies than single bond vibrations. (From Curry, Palings, Broek, Pardoen, Mulder, Lugtenburg, and Mathies, *J. Phys. Chem 88,* 688–702 (1984). The figure was kindly supplied by Prof. Richard Mathies, University of California, Berkeley.)

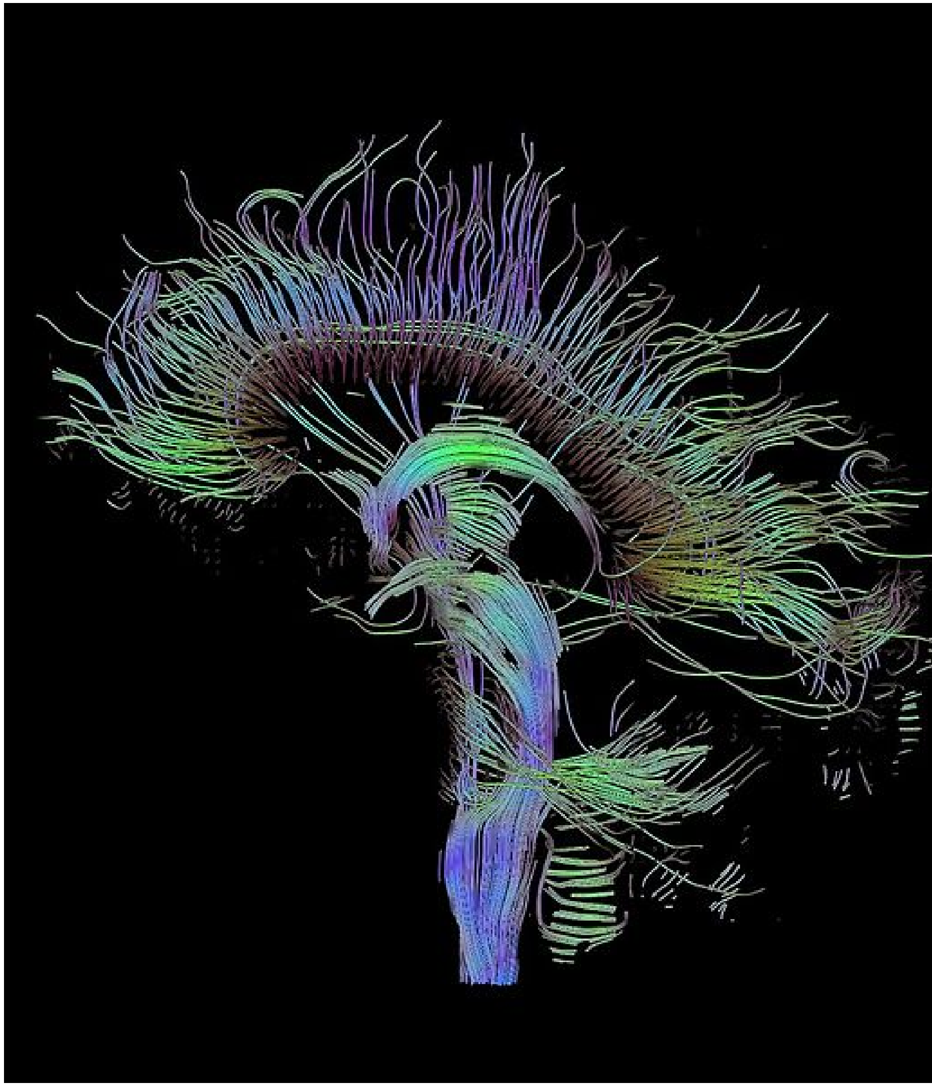
$C_7=C_8 + C_9=C_{10} + C_{11}=C_{12}$ Stretch.

361-16 Lec 40
Mon, 21nov16

NEW kinds of MRI (magnetic resononance imaging (MRI)
Diffusion Magnetic Resonance Imaging

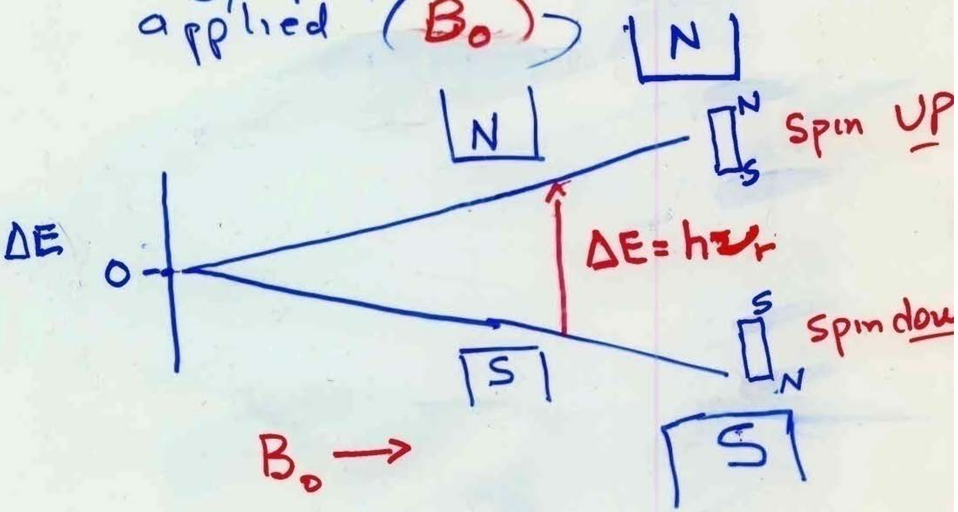


Tractographic reconstruction of neural connections via **Diffusion Tensor Imaging** (DTI)



MAGNETIC RESONANCE RECAP

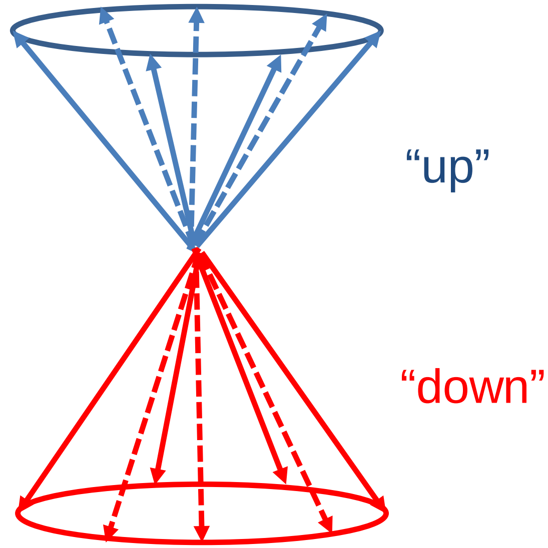
- Nuclear spins like bar magnets
- Electron & proton $\ell = 1/2$ spin
- Only 2 quantum states $m = +1/2, -1/2$ i.e., spin up & down
- Energy proportional to MAGNETIC FIELD applied (B_0)



ν_r = resonant frequency

- When $\nu = \nu_r$, radio frequency is ABSORBED

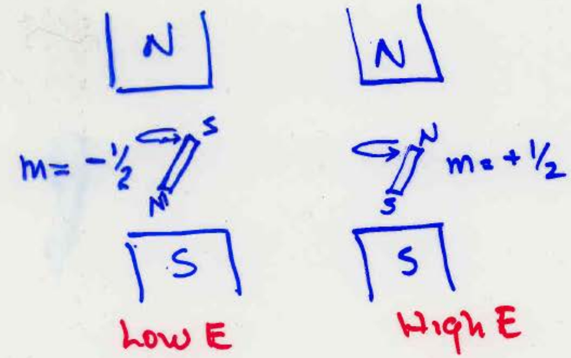
But what does "spin up" ***REALLY*** mean???

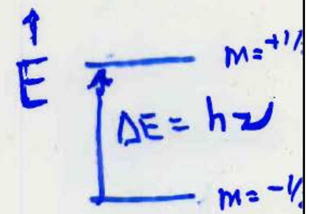


spin up and spin down are two quantum "energy levels" or STATIONARY STATES.

There is Equal Probability to observe any of the up arrows in the up state.

No spin ever points up!
But all lie on the cone so m=+1/2
The average vector points up



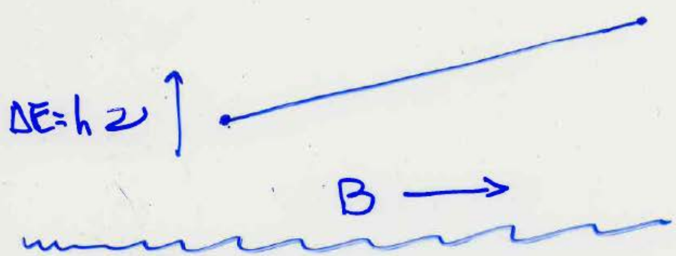


$$\Delta E = -\mu B_0 = h\nu$$

μ: magnetic dipole moment

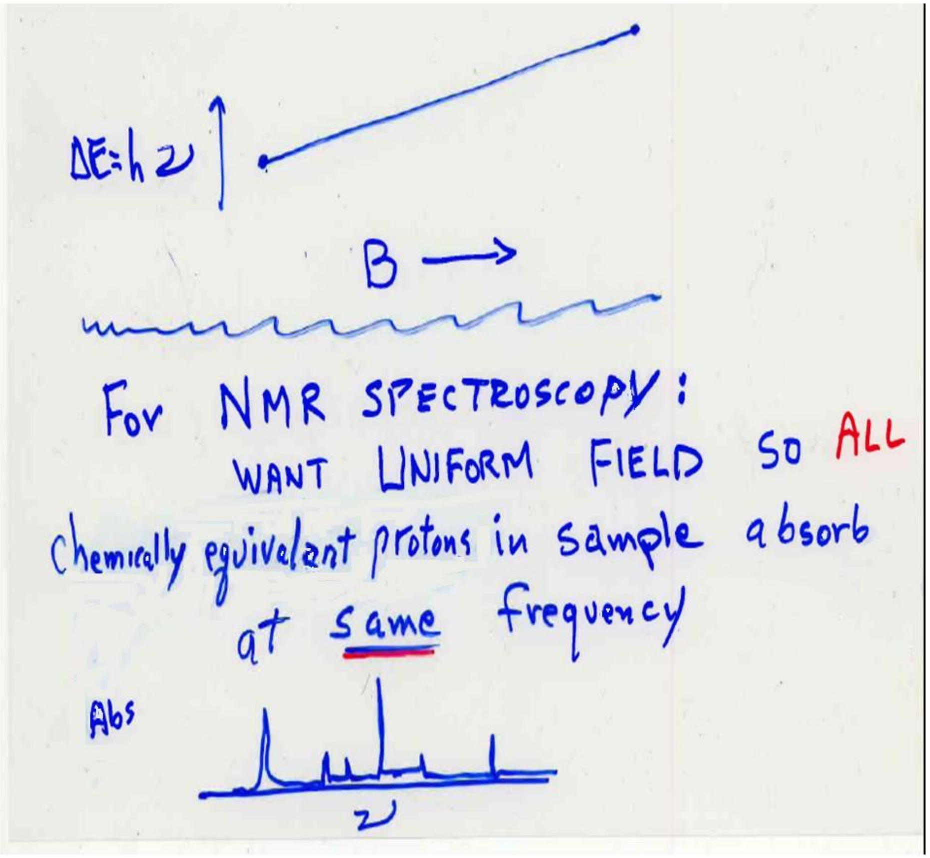
B_0: Field Strength.

So RESONANT FREQ ν, proportional to Field.



For NMR SPECTROSCOPY:
WANT UNIFORM FIELD SO ALL chemically equivalent protons in sample absorb at same frequency

NMR Spectroscopy vs. MRI:



The applied magnetic field is **<u>same everywhere in sample</u>.**

Field at the nucleus is **<u>reduced</u>** because of **<u>electron density</u>**
so **each chemically distinct H has a slightly different resonant frequency**
i.e., CHEMICAL SHIFT

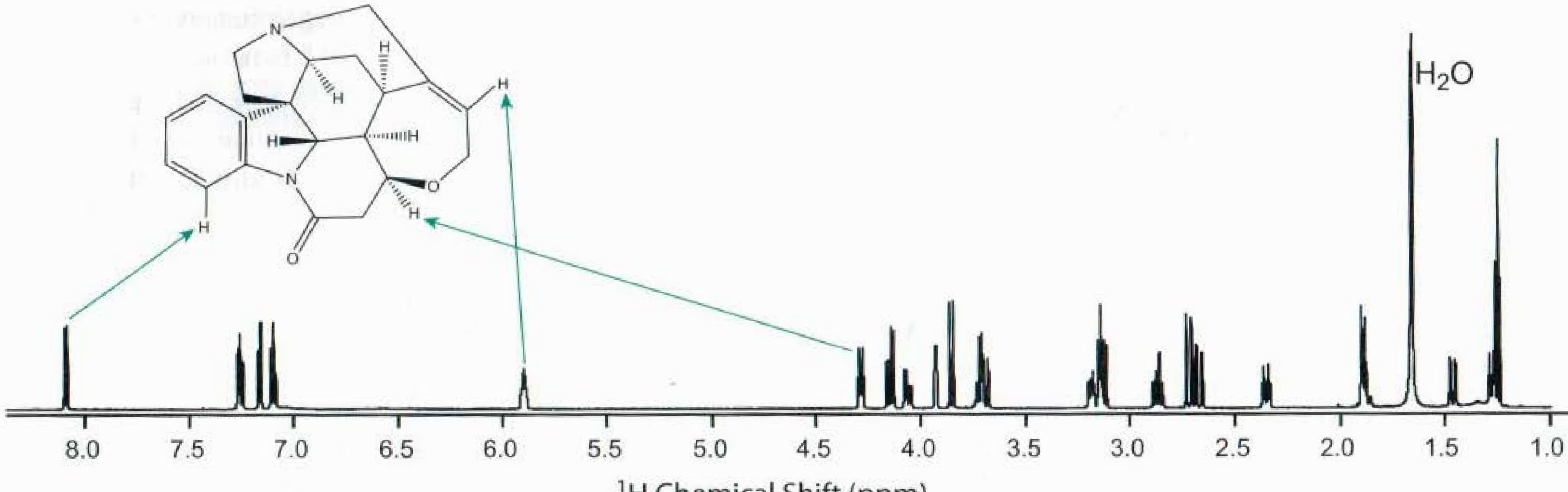


FIGURE 14.1 The [1]H NMR spectrum of strychnine (5 mM, 600 MHz) in deuterocholoroform ($CDCl_3$) illustrates the ability of NMR to obtain richly detailed information on complex molecules with atomic resolution. Each H atom gives a distinct signal with a characteristic position, splittings and relative intensity that is determined by the structure of the molecule. All signals are assigned, and a few representative assignments are shown on the figure (for clarity, not all H atoms are depicted). Complete assignments are performed with the aid of multidimensional NMR experiments. A residual signal from protonated chloroform ($CHCl_3$) has been digitally removed, while dissolved H_2O is noted.

For MRI (magnetic resonance imaging):

Applied **field is deliberately made to *vary* across the sample**.

Frequency set to **ONLY MEASURE WATER**

Then, **protons in different parts of sample will resonate at different frequency**

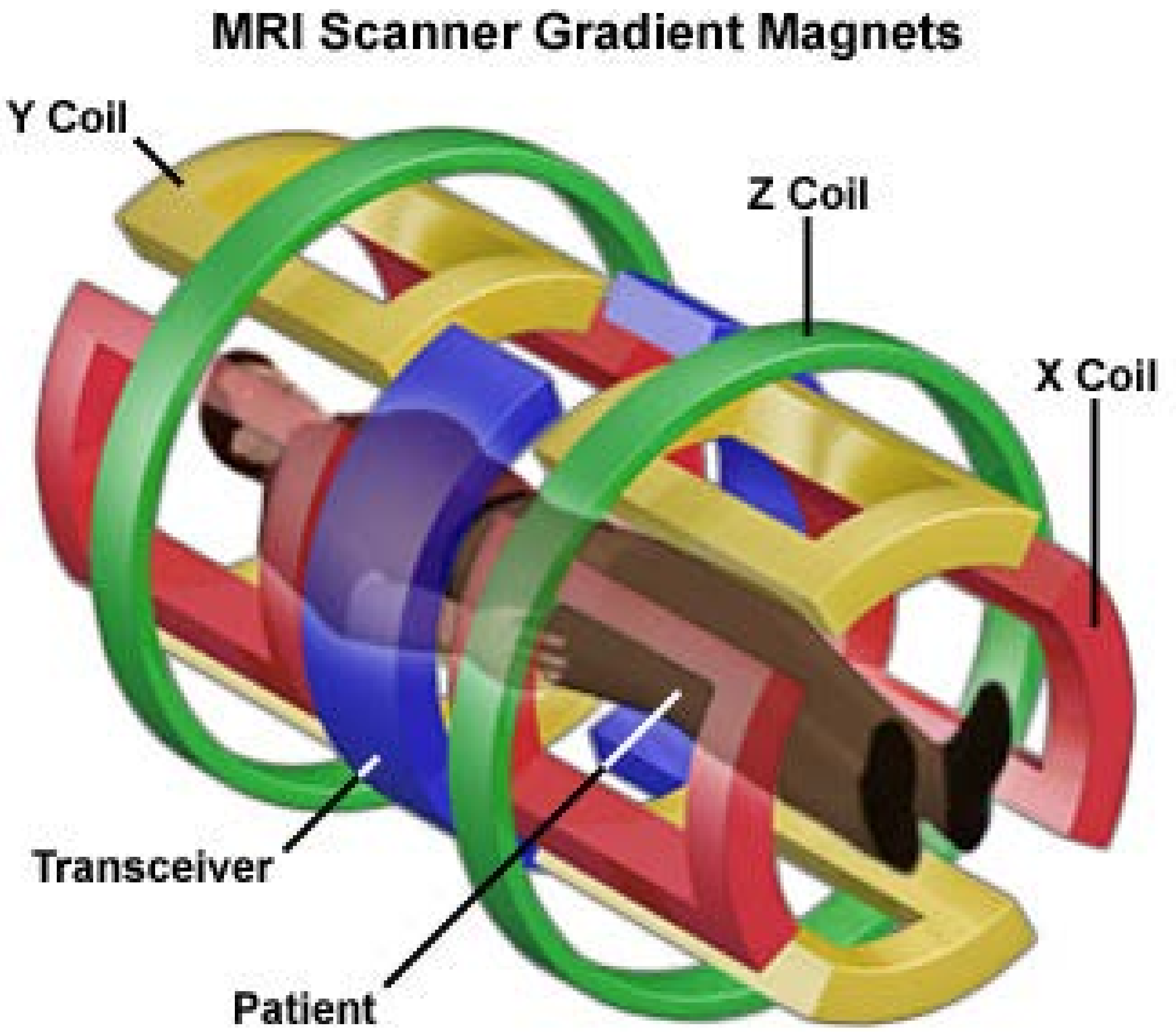
Only because of POSITION;

NOT because of different chemical shift

MRI Detects primarily two things:

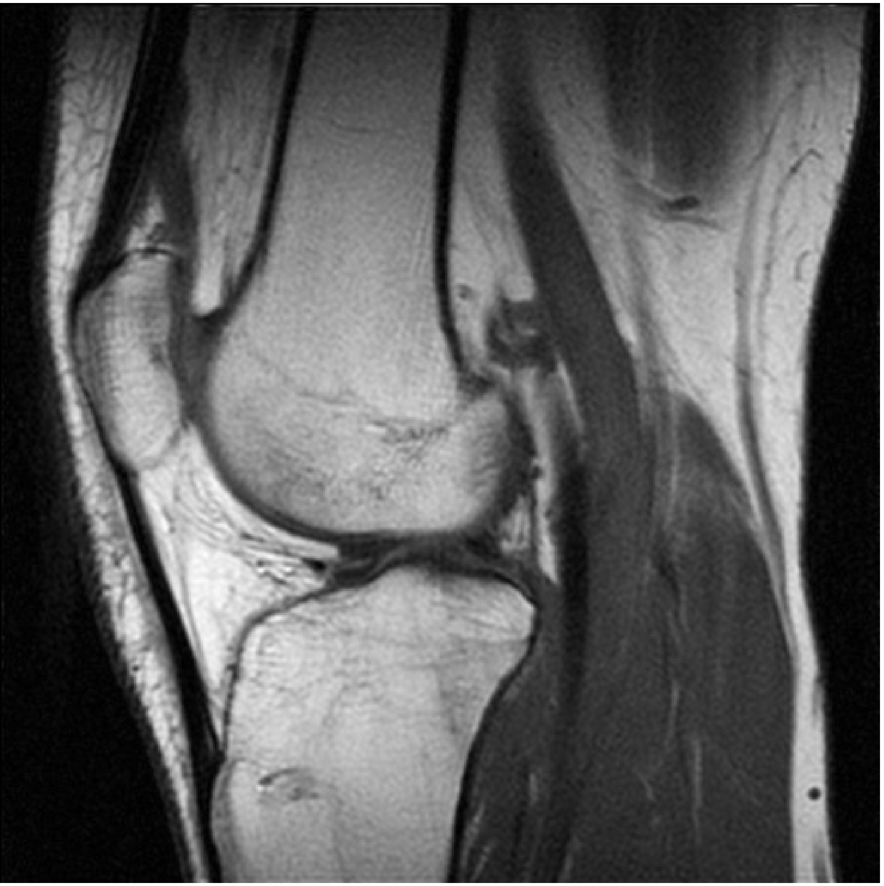
(1) **amount of water at different positions**

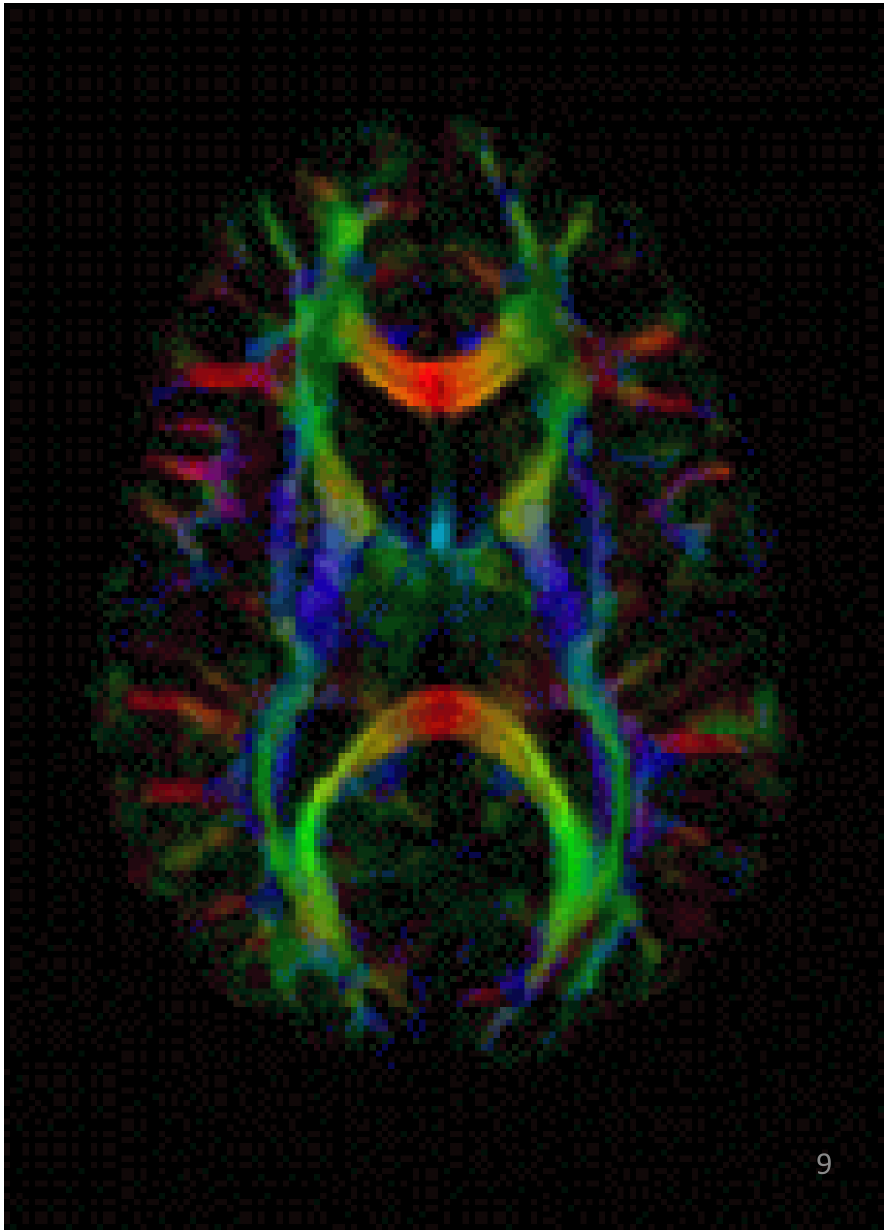
(2) and **direction of diffusion (more difficult)**

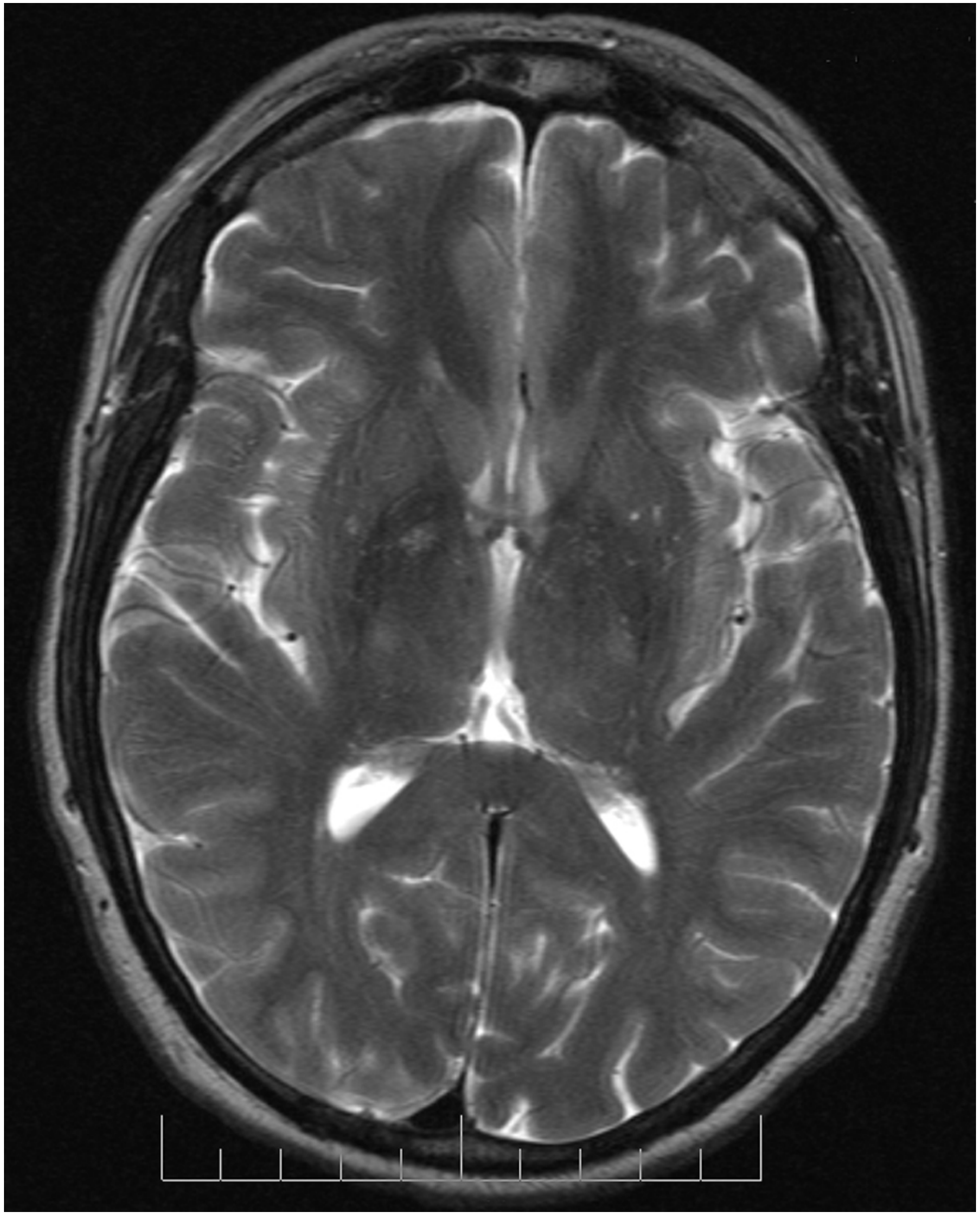

MRI Scanner Gradient Magnets
Y Coil
Z Coil
X Coil
Transceiver
Patient

diffusion tensor imaging (DTI)[

http://en.wikipedia.org/wiki/Magnetic_resonance_imaging







File:MRI T2 Brain axial image.jpg From Wikipedia, the free encyclopedia http://en.wikipedia.org/wiki/Magnetic_resonance_imaging

Magnetic resonance angiography (MRA) generates pictures of the arteries to evaluate them for stenosis (abnormal narrowing) or aneurysms

Using color to indicate frequency in different parts of the sample

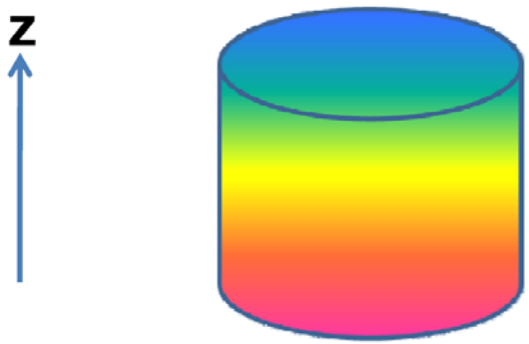
red is low frequency (because ***low*** field)
blue is high frequency (because ***high*** field)

Protons in different places absorb different frequencies.

Field increasing in x

x

Resonant frequency ν_r increasing in x



Field increasing in z

Resonant frequency ν_r increasing in z

But for MAGNETIC RESONANCE IMAGING (MRI)

FIELD HAS x or y or z GRADIENT

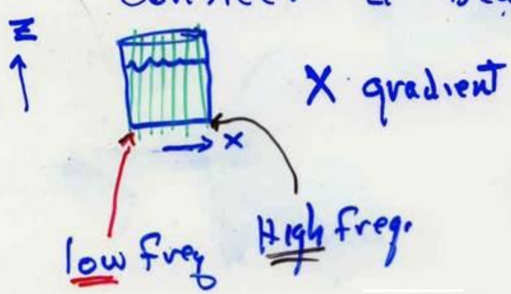
i.e. increases linearly as x or y or z increases.

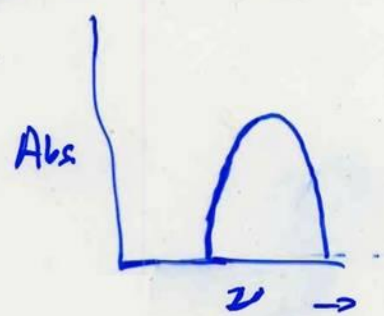
So ν also increases linearly as x or y or z increases

Different parts of sample resonate at different frequency.

Absorption strength depends on How many protons in resonance.

Consider a beaker of water

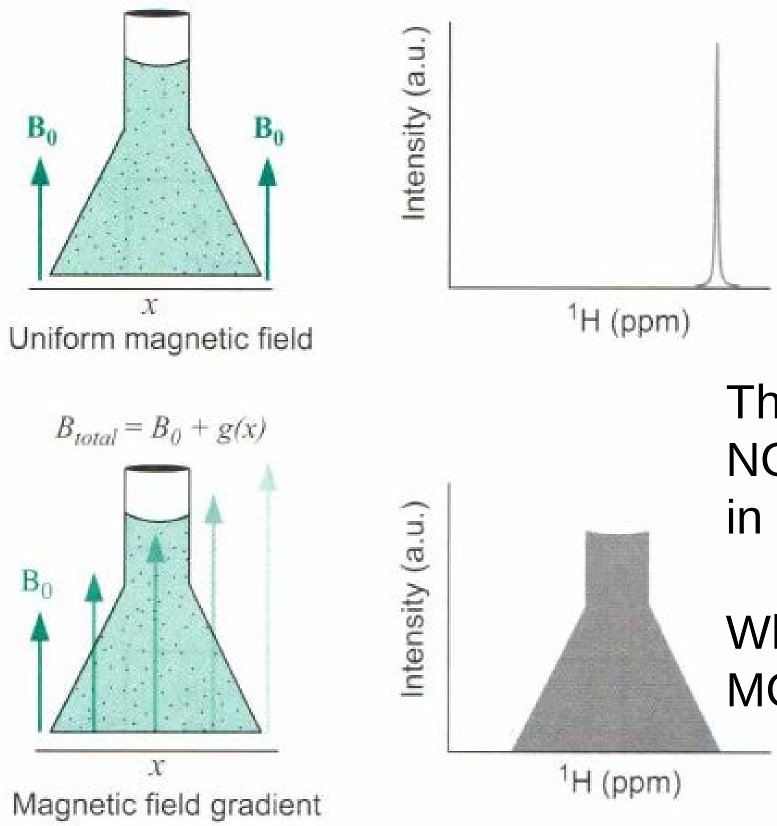




Abs proportial to amount of water in slices perpendicular to x

NMR

MRI



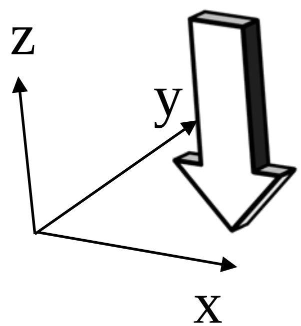
This image is
NOT CORRECT
in detail.

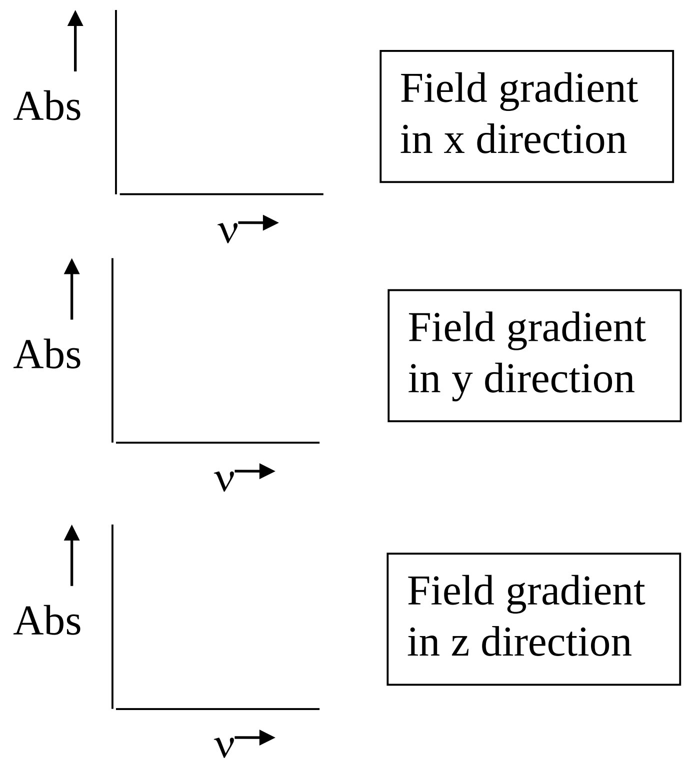
Which position has the
MOST water???

URE 14.29 Magnetic resonance imaging of a flask of water placed in a magnetic field that increases arly from left to right. A magnetic field gradient means that the resonance frequency of a proton ends on its position in the field. In a magnetic field gradient, a spectrum of intensity of absorption versus uency represents the number of protons versus position in the field. The spectrum is thus a projection of image of the water in the flask.

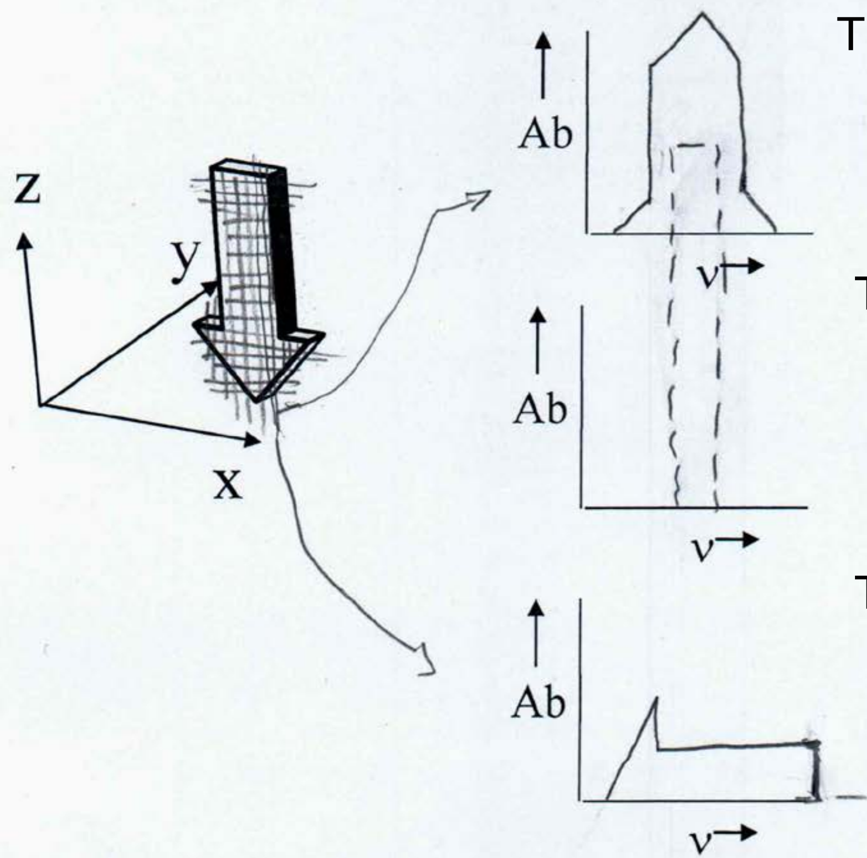
If the shape depicted below is filled with water, draw curves that indicate the intensity of absorbed radio frequency energy during an MRI of this object when the magnetic field gradient is in the x, y, z directions. (Field strength increases with increasing x, or y, or z.)

The long axis of the arrow is parallel to z. The plane of the arrow is perpendicular to the y axis.





(11 pts) 9. If the shape depicted below is filled with water, draw curves that indicate the intensity of absorbed radio frequency energy during an MRI of this object when the magnetic field gradient is in the x, y, z directions. (Field strength increases with increasing x, or y, or z.)
The long axis of the arrow is parallel to z. The plane of the arrow is perpendicular to the y axis.



Think: **Vertical slices perp. to X**

Field gradient in x direction

Think: **Vertical slices perp. to Y**

Field gradient in y direction

Think: **Vertical slices perp. to Z**

Field gradient in z direction